Electronic Supplementary Material (ESI) for RSC Advances.
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Pyrazolone-type compounds (part II): *In vitro* and *in silico* evaluation of antioxidant potential; structure-activity relationship

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Table S1 Calculated stabilization energies (kJ mol $^{-1}$) for compounds **a**–**t** in water.

	Ring A		Ring B		Ring C		
ΔE_{iso} (kJ mol $^{-1}$)	N1	N2	O1	N2	O1	O2	O3
Compound							
a	-7.95	-21.60	0.29	26.91	/	/	/
b	-7.10	-22.46	-3.53	26.19	-7.78	/	/
c	-8.15	-22.01	-1.23	26.60	/	-2.63	/
d	-8.05	-21.70	0.91	27.16	/	/	-9.76
e	-7.44	-20.46	0.81	27.07	/	/	/
f	-7.26	-20.47	1.19	27.66	/	/	/
g	-7.53	-20.88	-1.54	27.46	/	/	/
h	-3.00	-15.21	0.20	31.57	/	/	/
i	-6.42	-19.38	2.26	27.85	/	/	/
j	-6.17	-18.90	1.55	29.00	/	/	/
k	-5.60	-18.20	-1.98	31.77	/	/	/
l	-5.57	-19.94	3.39	28.93	/	/	/
m	-6.56	-19.50	-4.30	27.55	-34.76	-30.78	/
n	-7.64	-21.27	0.71	26.41	/	-35.18	-35.44
o	-7.20	-23.79	-3.10	26.44	-25.51	/	/
p	-8.78	-22.33	0.84	25.52	/	/	-28.27
q	-7.57	-21.26	1.58	27.19	/	/	-43.93
r	-8.09	-21.05	1.29	26.88	/	-16.48	/
s	-7.57	-21.19	1.35	26.70	/	/	/
t	-6.06	-19.79	-1.83	27.85	-12.23	/	/

Table S2 Calculated stabilization energies (kJ mol $^{-1}$) for compounds **a**–**t** in benzene.

	Ring A		Ring B		Ring C		
ΔE_{iso} (kJ mol $^{-1}$)	N1	N2	O1	N2	O1	O2	O3
Compound							
a	-7.98	-35.72	-4.55	31.36	/	/	/
b	-7.37	-35.50	-8.02	29.77	-13.82	/	/
c	-8.23	-36.20	-5.43	31.06	/	-1.35	/
d	-8.12	-35.98	-3.49	30.90	/	/	-7.92
e	-6.49	-33.74	-2.71	32.35	/	/	/
f	-7.19	-34.52	-3.99	32.42	/	/	/
g	-7.43	-34.86	12.89	32.13	/	/	/
h	-5.53	-29.04	16.55	33.13	/	/	/
i	-2.75	-29.33	-3.55	38.83	/	/	/
j	-5.99	-32.55	-3.21	34.47	/	/	/
k	-7.41	-34.42	-9.60	31.49	/	/	/
l	-8.31	-36.47	-4.26	30.78	/	/	/
m	-6.65	-33.73	11.86	32.72	-44.08	-37.39	/
n	-8.58	-36.12	-6.07	31.15	/	-37.44	-41.59
o	-7.89	-35.50	-6.87	29.25	-19.03	/	/
p	-7.88	-35.77	20.93	30.80	/	/	-14.03
q	-8.81	-36.85	-5.95	30.76	/	/	-30.31
r	-7.14	-34.82	20.29	28.57	/	-18.55	/
s	-8.15	-36.52	-5.56	30.48	/	/	/
t	-5.71	-32.82	-7.51	32.94	-13.19	/	/

Table S3. Calculated bond dissociation enthalpies (kJ mol $^{-1}$) for compounds **a–t** in water.

	Bond dissociation enthalpy (BDE) kJ/mol						
	N1 (A)	N2 (A)	O1 (B)	N2 (B)	O1 (C)	O2 (C)	O3 (C)
a	342	329	351	377	/	/	/
b	343	328	347	377	343	/	/
c	342	328	349	377	/	348	/
d	342	329	351	378	/	/	341
e	343	330	351	377	/	/	/
f	343	330	352	378	/	/	/
g	343	329	349	378	/	/	/
h	347	335	351	382	/	/	/
i	344	331	353	378	/	/	/
j	344	331	352	379	/	/	/
k	345	332	348	382	/	/	/
l	345	330	354	379	/	/	/
m	344	331	346	378	316	320	/
n	343	329	351	377	/	315	315
o	343	327	347	377	325	/	/
p	342	328	351	376	/	/	322
q	343	329	352	378	/	/	306
r	342	329	352	377	/	334	/
s	343	329	352	377	/	/	/
t	344	331	349	378	338	/	/

Table S4 Calculated IP and PDE values (kJ mol $^{-1}$) for compounds **a–t** in water.

kJ/mol	SET-PT							
	IP	PDE						
		N1 (A)	N2 (A)	O1 (B)	N2 (B)	O2 (C)	O3 (C)	O4 (C)
a	435	62	49	71	97	/	/	/
b	433	65	49	68	98	64	/	/
c	435	62	48	68	96	/	67	/
d	443	54	40	63	89	/	/	52
e	437	60	47	69	95	/	/	/
f	437	61	48	69	96	/	/	/
g	436	41	48	67	96	/	/	/
h	441	60	48	64	95	/	/	/
i	439	59	46	68	94	/	/	/
j	440	58	49	66	93	/	/	/
k	437	63	50	66	100	/	/	/
l	436	63	49	72	97	/	/	/
m	438	60	47	62	94	32	36	/
n	428	69	55	77	103	/	41	41
o	431	66	50	70	100	48	/	/
p	421	75	61	84	109	/	/	55
q	416	81	68	91	116	/	/	45
r	435	61	48	71	96	/	53	/
s	418	80	66	89	114	/	/	/
t	410	89	75	93	123	83	/	/

Table S5. Calculated PA and ETE values (kJ mol -1) for compounds a–t in water.

kJ/mol	SPLET													
	N1 (A)		N2 (A)		O1 (B)		N2 (B)		O1 (C)		O2 (C)		O3 (C)	
	PA	ETE	PA	ETE	PA	ETE	PA	ETE	PA	ETE	PA	ETE	PA	ETE
a	144	353	140	343	181	324	203	329	/	/	/	/	/	/
b	143	355	138	344	174	327	202	329	159	338	/	/	/	/
c	144	353	139	343	181	322	203	328	/	/	161	341	/	/
d	145	352	140	343	181	324	203	329	/	/	/	/	162	333
e	142	355	138	346	180	326	201	330	/	/	/	/	/	/
f	141	357	139	345	180	326	199	333	/	/	/	/	/	/
g	141	356	139	345	180	323	202	330	/	/	/	/	/	/
h	141	360	136	353	174	331	201	335	/	/	/	/	/	/
i	142	357	137	348	179	328	201	332	/	/	/	/	/	/
j	141	357	137	349	177	329	200	334	/	/	/	/	/	/
k	147	352	142	344	179	323	205	332	/	/	/	/	/	/
l	147	352	142	343	184	324	206	328	/	/	/	/	/	/
m	145	354	139	347	178	323	203	330	143	327	144	330	/	/
n	144	353	140	344	182	324	203	328	/	/	146	324	147	323
o	144	354	139	342	175	327	203	329	162	318	/	/	/	/
p	144	352	140	343	182	324	203	328	/	/	/	/	162	314
q	144	353	140	343	184	322	203	329	/	/	/	/	162	299
r	142	355	139	344	181	325	202	330	/	/	152	336	/	/
s	144	354	139	344	181	325	202	329	/	/	/	/	/	/
t	141	358	136	349	172	331	200	332	136	356	/	/	/	/

Table S6. Calculated bond dissociation enthalpies (kJ mol $^{-1}$) for compounds **a–t** in benzene.

	Bond dissociation enthalpy (BDE) kJ/mol						
	N1 (A)	N2 (A)	O1 (B)	N2 (B)	O1 (C)	O2 (C)	O3 (C)
a	340	313	344	380	/	/	/
b	341	313	340	378	334	/	/
c	340	312	343	379	/	347	/
d	340	312	345	379	/	/	345
e	342	315	346	381	/	/	/
f	341	314	344	381	/	/	/
g	341	313	361	380	/	/	/
h	343	319	365	381	/	/	/
i	364	319	345	387	/	/	/
j	342	316	345	383	/	/	/
k	341	314	339	380	/	/	/
l	340	312	344	379	/	/	/
m	342	315	360	381	304	311	/
n	340	312	342	379	/	311	307
o	340	313	314	378	329	/	/
p	340	312	369	379	/	/	334
q	339	311	342	379	/	/	318
r	341	313	369	377	/	330	/
s	340	312	343	379	/	/	/
t	343	315	341	381	335	/	/

Table S7 Calculated IP and PDE values (kJ mol $^{-1}$) for compounds **a–t** in benzene.

kJ/mol	SET-PT							
	IP	PDE						
		N1 (A)	N2 (A)	O1 (B)	N2 (B)	O1 (C)	O2 (C)	O3 (C)
a	551	178	151	182	218	/	/	/
b	544	186	158	186	223	180	/	/
c	549	180	152	183	220	/	187	/
d	550	179	151	184	218	/	/	179
e	557	174	147	178	213	/	/	/
f	557	173	146	176	213	/	/	/
g	556	174	146	194	213	/	/	/
h	558	174	150	196	212	/	/	/
i	567	167	141	167	209	/	/	/
j	568	164	137	167	204	/	/	/
k	553	178	151	175	216	/	/	/
l	550	179	151	183	219	/	/	/
m	543	187	160	206	227	150	157	/
n	547	182	154	184	221	/	153	149
o	540	190	162	191	227	179	/	/
p	573	157	129	186	196	/	/	151
q	558	171	143	174	210	/	/	149
r	553	177	150	205	213	/	166	/
s	549	180	152	183	219	/	/	/
t	555	177	150	175	216	170	/	/

Table S8. Calculated PA and ETE values (kJ mol $^{-1}$) for compounds **a–t** in benzene.

kJ/mol	SPLET													
	N1 (A)		N2 (A)		O1 (B)		N2 (B)		O1 (C)		O2 (C)		O3 (C)	
	PA	ETE	PA	ETE	PA	ETE	PA	ETE	PA	ETE	PA	ETE	PA	ETE
a	393	337	363	338	495	238	463	306	/	/	/	/	/	/
b	395	335	368	334	450	279	467	301	408	316	/	/	/	/
c	393	336	364	338	446	286	465	304	/	/	431	305	/	/
d	393	336	364	337	495	239	463	306	/	/	/	/	436	294
e	388	343	358	345	488	247	457	313	/	/	/	/	/	/
f	386	344	355	348	487	246	457	313	/	/	/	/	/	/
g	388	342	359	344	489	262	458	311	/	/	/	/	/	/
h	385	347	360	348	442	312	454	317	/	/	/	/	/	/
i	380	355	351	357	479	255	458	318	/	/	/	/	/	/
j	376	355	347	358	472	262	448	324	/	/	/	/	/	/
k	392	338	362	341	487	241	463	306	/	/	/	/	/	/
l	394	335	365	336	496	238	463	305	/	/	/	/	/	/
m	394	337	365	339	454	295	475	296	384	309	394	306	/	/
n	393	336	363	338	447	284	466	302	/	/	403	297	403	292
o	397	332	371	331	457	274	469	298	428	291	/	/	/	/
p	389	341	365	337	493	266	459	309	/	/	/	/	455	268
q	389	340	360	341	439	293	461	308	/	/	/	/	459	248
r	390	340	363	340	491	267	458	308	/	/	427	292	/	/
s	390	340	360	341	494	238	459	309	/	/	/	/	/	/
t	385	347	357	347	439	291	457	313	377	348	/	/	/	/

Table S9. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **a** with the selected radical species in methanol.

a		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	80	-161	-73	-8
	N2 (A)	-95		-175	-78	-17
	N2 (B)	-46		-126	-15	-32
	O1 (B)	-75		-155	-36	-39
$\cdot OC(CH_3)_3$	N1 (A)	-89	80	-169	-81	-8
	N2 (A)	-104		-184	-87	-16
	N2 (B)	-55		-135	-23	-31
	O1 (B)	-84		-164	-45	-39
$\cdot OH$	N1 (A)	-152	1	-153	-65	-87
	N2 (A)	-167		-168	-71	-96
	N2 (B)	-118		-119	-7	-110
	O1 (B)	-147		-148	-29	-118
$\cdot OOH$	N1 (A)	-12	102	-115	-26	14
	N2 (A)	-27		-129	-32	6
	N2 (B)	22		-80	31	-9
	O1 (B)	-7		-109	10	-17
$\cdot OOCH_3$	N1 (A)	-5	111	-116	-28	23
	N2 (A)	-19		-131	-34	14
	N2 (B)	30		-82	30	0
	O1 (B)	0		-111	9	-8
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	92	-96	-8	3
	N2 (A)	-19		-111	-14	-5
	N2 (B)	30		-62	50	-20
	O1 (B)	1		-91	29	-28
DPPH	N1 (A)	24	80	-56	33	-9
	N2 (A)	9		-70	27	-17
	N2 (B)	58		-21	90	-32
	O1 (B)	29		-50	69	-40
$O_2^{\cdot -}$	N1 (A)	60	269	-209	46	14
	N2 (A)	45		-224	40	6
	N2 (B)	94		-175	103	-9
	O1 (B)	65		-204	82	-17

Table S10. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **b** with the selected radical species in methanol.

b		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	79	-159	-73	-7
	N2 (A)	-96		-175	-80	-16
	N2 (B)	-50		-129	-13	-37
	O1 (B)	-78		-157	-43	-36
	O1 (C)	-83		-162	-59	-23
$\cdot OC(CH_3)_3$	N1 (A)	-88	79	-168	-82	-6
	N2 (A)	-104		-184	-88	-16
	N2 (B)	-58		-137	-21	-37
	O1 (B)	-87		-166	-51	-35
	O1 (C)	-91		-170	-68	-23
$\cdot OH$	N1 (A)	-151	0	-152	-66	-86
	N2 (A)	-167		-167	-72	-95
	N2 (B)	-121		-121	-5	-116
	O1 (B)	-150		-150	-35	-115
	O1 (C)	-154		-154	-52	-102
$\cdot OOH$	N1 (A)	-11	101	-113	-27	16
	N2 (A)	-27		-129	-34	6
	N2 (B)	19		-83	33	-15
	O1 (B)	-10		-111	4	-13
	O1 (C)	-14		-116	-13	-1
$\cdot OOCH_3$	N1 (A)	-4	110	-114	-29	24
	N2 (A)	-20		-130	-35	15
	N2 (B)	26		-84	32	-6
	O1 (B)	-3		-113	2	-5
	O1 (C)	-7		-117	-15	8
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	91	-94	-9	5
	N2 (A)	-20		-110	-15	-5
	N2 (B)	27		-64	52	-26
	O1 (B)	-2		-93	22	-24
	O1 (C)	-7		-97	5	-12
DPPH	N1 (A)	25	79	-54	32	-7
	N2 (A)	9		-70	25	-17
	N2 (B)	55		-24	92	-38
	O1 (B)	26		-52	62	-36
	O1 (C)	22		-57	46	-24
$O_2^{\cdot -}$	N1 (A)	61	268	-207	45	16
	N2 (A)	45		-223	38	6
	N2 (B)	91		-177	105	-15
	O1 (B)	62		-206	76	-13
	O1 (C)	58		-210	59	-1

Table S11. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **c** with the selected radical species in methanol.

c		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	81	-162	-72	-8
	N2 (A)	-95		-176	-79	-17
	N2 (B)	-46		-127	-12	-34
	O1 (B)	-75		-155	-35	-39
	O2 (C)	-77		-158	-57	-21
$\cdot OC(CH_3)_3$	N1 (A)	-89	81	-170	-81	-8
	N2 (A)	-104		-185	-87	-16
	N2 (B)	-54		-136	-21	-34
	O1 (B)	-83		-164	-44	-39
	O2 (C)	-86		-167	-65	-20
$\cdot OH$	N1 (A)	-152	2	-154	-65	-87
	N2 (A)	-167		-169	-71	-96
	N2 (B)	-118		-120	-5	-113
	O1 (B)	-146		-148	-28	-118
	O2 (C)	-149		-151	-49	-100
$\cdot OOH$	N1 (A)	-12	103	-115	-26	14
	N2 (A)	-27		-130	-33	6
	N2 (B)	22		-81	34	-12
	O1 (B)	-6		-109	11	-17
	O2 (C)	-9		-112	-10	2
$\cdot OOCH_3$	N1 (A)	-5	112	-117	-27	23
	N2 (A)	-20		-132	-34	14
	N2 (B)	30		-82	33	-3
	O1 (B)	1		-111	9	-8
	O2 (C)	-1		-113	-12	10
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	92	-97	-7	3
	N2 (A)	-19		-112	-14	-5
	N2 (B)	30		-62	53	-23
	O1 (B)	2		-91	29	-28
	O2 (C)	-1		-93	8	-9
DPPH	N1 (A)	24	80	-56	33	-9
	N2 (A)	9		-71	26	-17
	N2 (B)	58		-22	93	-35
	O1 (B)	30		-50	70	-40
	O2 (C)	27		-53	48	-21
$O_2^{\cdot -}$	N1 (A)	60	270	-210	46	14
	N2 (A)	45		-225	39	6
	N2 (B)	94		-175	106	-12
	O1 (B)	66		-204	83	-17
	O2 (C)	63		-207	62	2

Table S12. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **d** with the selected radical species in methanol.

d		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	89	-169	-72	-9
	N2 (A)	-95		-184	-78	-17
	N2 (B)	-45		-134	-12	-33
	O1 (B)	-74		-163	-35	-40
	O3 (C)	-84		-173	-56	-29
$\cdot OC(CH_3)_3$	N1 (A)	-89	89	-178	-80	-8
	N2 (A)	-103		-192	-86	-17
	N2 (B)	-54		-143	-21	-33
	O1 (B)	-83		-172	-43	-39
	O3 (C)	-93		-182	-64	-28
$\cdot OH$	N1 (A)	-152	10	-162	-64	-88
	N2 (A)	-166		-176	-70	-96
	N2 (B)	-117		-127	-5	-112
	O1 (B)	-146		-156	-27	-119
	O3 (C)	-156		-166	-48	-108
$\cdot OOH$	N1 (A)	-12	111	-123	-25	14
	N2 (A)	-26		-138	-32	5
	N2 (B)	23		-88	34	-11
	O1 (B)	-6		-117	11	-17
	O3 (C)	-16		-127	-10	-6
$\cdot OOCH_3$	N1 (A)	-5	120	-124	-27	22
	N2 (A)	-19		-139	-33	14
	N2 (B)	30		-89	33	-2
	O1 (B)	1		-118	10	-9
	O3 (C)	-9		-128	-11	2
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	100	-104	-7	3
	N2 (A)	-19		-119	-13	-6
	N2 (B)	31		-69	53	-22
	O1 (B)	2		-98	30	-28
	O3 (C)	-8		-108	9	-17
DPPH	N1 (A)	24	88	-64	33	-9
	N2 (A)	10		-79	27	-18
	N2 (B)	59		-29	93	-34
	O1 (B)	30		-58	70	-40
	O3 (C)	20		-68	49	-29
$O_2^{\cdot -}$	N1 (A)	60	278	-218	47	14
	N2 (A)	46		-232	40	5
	N2 (B)	95		-183	106	-11
	O1 (B)	66		-212	83	-17
	O3 (C)	56		-222	62	-6

Table S13. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **e** with the selected radical species in methanol.

e		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	83	-163	-74	-6
	N2 (A)	-94		-177	-80	-14
	N2 (B)	-46		-129	-14	-32
	O1 (B)	-75		-158	-37	-37
$\cdot OC(CH_3)_3$	N1 (A)	-88	83	-171	-83	-5
	N2 (A)	-102		-185	-89	-14
	N2 (B)	-54		-137	-22	-32
	O1 (B)	-83		-166	-46	-37
$\cdot OH$	N1 (A)	-151	4	-155	-67	-85
	N2 (A)	-165		-169	-73	-93
	N2 (B)	-117		-121	-6	-111
	O1 (B)	-146		-150	-30	-116
$\cdot OOH$	N1 (A)	-11	105	-117	-28	17
	N2 (A)	-25		-131	-34	8
	N2 (B)	23		-82	32	-10
	O1 (B)	-6		-112	9	-15
$\cdot OOCH_3$	N1 (A)	-4	114	-118	-29	25
	N2 (A)	-18		-132	-35	17
	N2 (B)	30		-84	31	-1
	O1 (B)	1		-113	7	-6
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	94	-98	-9	6
	N2 (A)	-18		-112	-15	-2
	N2 (B)	31		-64	51	-20
	O1 (B)	1		-93	27	-26
DPPH	N1 (A)	25	82	-58	31	-6
	N2 (A)	11		-72	25	-15
	N2 (B)	59		-23	91	-32
	O1 (B)	30		-53	68	-38
$O_2\cdot^-$	N1 (A)	61	272	-211	44	17
	N2 (A)	47		-225	38	8
	N2 (B)	95		-177	104	-10
	O1 (B)	66		-206	81	-15

Table S14. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **f** with the selected radical species in methanol.

f		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	83	-163	-73	-7
	N2 (A)	-94		-177	-79	-15
	N2 (B)	-45		-128	-14	-31
	O1 (B)	-74		-157	-37	-38
$\cdot OC(CH_3)_3$	N1 (A)	-88	83	-171	-82	-6
	N2 (A)	-102		-185	-88	-14
	N2 (B)	-53		-137	-22	-31
	O1 (B)	-82		-166	-45	-37
$\cdot OH$	N1 (A)	-151	4	-155	-66	-85
	N2 (A)	-165		-169	-72	-94
	N2 (B)	-117		-121	-6	-110
	O1 (B)	-146		-150	-29	-116
$\cdot OOH$	N1 (A)	-11	105	-116	-27	16
	N2 (A)	-25		-131	-33	8
	N2 (B)	23		-82	32	-9
	O1 (B)	-6		-111	10	-15
$\cdot OOCH_3$	N1 (A)	-4	114	-118	-28	24
	N2 (A)	-18		-132	-34	16
	N2 (B)	31		-83	31	0
	O1 (B)	2		-112	8	-6
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-3	94	-98	-8	5
	N2 (A)	-18		-112	-14	-3
	N2 (B)	31		-63	51	-20
	O1 (B)	2		-92	28	-26
DPPH	N1 (A)	25	82	-57	32	-7
	N2 (A)	11		-72	26	-15
	N2 (B)	59		-23	91	-32
	O1 (B)	30		-52	68	-38
$O_2^{\cdot -}$	N1 (A)	61	272	-211	45	16
	N2 (A)	47		-225	39	8
	N2 (B)	95		-176	104	-9
	O1 (B)	66		-206	82	-15

Table S15. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **g** with the selected radical species in methanol.

g		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	82	-162	-73	-7
	N2 (A)	-94		-176	-79	-15
	N2 (B)	-45		-127	-13	-32
	O1 (B)	-74		-157	-36	-38
$\cdot OC(CH_3)_3$	N1 (A)	-88	83	-171	-81	-7
	N2 (A)	-103		-185	-88	-15
	N2 (B)	-54		-136	-22	-32
	O1 (B)	-83		-165	-45	-38
$\cdot OH$	N1 (A)	-151	3	-155	-65	-86
	N2 (A)	-166		-169	-72	-94
	N2 (B)	-117		-120	-6	-111
	O1 (B)	-146		-149	-29	-117
$\cdot OOH$	N1 (A)	-11	105	-116	-27	15
	N2 (A)	-26		-130	-33	7
	N2 (B)	23		-81	33	-9
	O1 (B)	-6		-110	10	-16
$\cdot OOCH_3$	N1 (A)	-4	113	-117	-28	24
	N2 (A)	-18		-132	-34	16
	N2 (B)	31		-83	31	-1
	O1 (B)	1		-112	8	-7
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	94	-97	-8	4
	N2 (A)	-18		-112	-14	-4
	N2 (B)	31		-63	51	-20
	O1 (B)	2		-92	28	-27
DPPH	N1 (A)	25	82	-57	32	-8
	N2 (A)	10		-71	26	-16
	N2 (B)	59		-22	92	-32
	O1 (B)	30		-52	69	-39
$O_2\cdot^-$	N1 (A)	61	271	-210	45	15
	N2 (A)	46		-225	39	7
	N2 (B)	95		-176	105	-9
	O1 (B)	66		-205	82	-16

Table S16. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **h** with the selected radical species in methanol.

h		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-77	86	-163	-77	0
	N2 (A)	-91		-176	-84	-7
	N2 (B)	-44		-129	-16	-27
	O1 (B)	-77		-163	-45	-32
$\cdot OC(CH_3)_3$	N1 (A)	-85	86	-171	-86	0
	N2 (A)	-99		-185	-92	-7
	N2 (B)	-52		-138	-25	-27
	O1 (B)	-85		-171	-54	-31
$\cdot OH$	N1 (A)	-149	7	-155	-70	-79
	N2 (A)	-162		-169	-76	-86
	N2 (B)	-115		-122	-9	-106
	O1 (B)	-148		-155	-38	-111
$\cdot OOH$	N1 (A)	-9	108	-117	-31	22
	N2 (A)	-22		-130	-37	15
	N2 (B)	25		-83	30	-5
	O1 (B)	-8		-116	1	-9
$\cdot OOCH_3$	N1 (A)	-1	117	-118	-32	31
	N2 (A)	-15		-131	-39	24
	N2 (B)	32		-84	29	4
	O1 (B)	-1		-118	-1	-1
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	97	-98	-12	11
	N2 (A)	-14		-111	-19	4
	N2 (B)	33		-64	49	-16
	O1 (B)	-1		-98	19	-20
DPPH	N1 (A)	27	85	-58	28	-1
	N2 (A)	14		-71	21	-8
	N2 (B)	61		-24	89	-28
	O1 (B)	28		-57	60	-32
$O_2^{\cdot -}$	N1 (A)	63	274	-211	41	22
	N2 (A)	50		-225	35	15
	N2 (B)	97		-178	102	-5
	O1 (B)	64		-211	73	-9

Table S17. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **i** with the selected radical species in methanol.

i		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-77	88	-164	-73	-4
	N2 (A)	-91		-178	-79	-11
	N2 (B)	-42		-130	-13	-30
	O1 (B)	-71		-158	-36	-35
$\cdot OC(CH_3)_3$	N1 (A)	-85	88	-173	-82	-3
	N2 (A)	-99		-187	-88	-11
	N2 (B)	-51		-139	-21	-29
	O1 (B)	-79		-167	-45	-34
$\cdot OH$	N1 (A)	-148	9	-157	-66	-83
	N2 (A)	-162		-171	-72	-90
	N2 (B)	-114		-123	-5	-109
	O1 (B)	-142		-151	-29	-114
$\cdot OOH$	N1 (A)	-8	110	-118	-27	19
	N2 (A)	-22		-132	-33	11
	N2 (B)	26		-84	34	-7
	O1 (B)	-2		-112	10	-12
$\cdot OOCH_3$	N1 (A)	-1	119	-120	-28	27
	N2 (A)	-15		-133	-34	20
	N2 (B)	33		-85	32	1
	O1 (B)	5		-114	9	-4
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	99	-100	-8	8
	N2 (A)	-14		-113	-14	0
	N2 (B)	34		-65	52	-18
	O1 (B)	5		-94	29	-23
DPPH	N1 (A)	28	87	-59	32	-4
	N2 (A)	14		-73	26	-12
	N2 (B)	62		-25	92	-30
	O1 (B)	34		-53	69	-35
$O_2\cdot^-$	N1 (A)	64	277	-213	45	19
	N2 (A)	50		-227	39	11
	N2 (B)	98		-178	106	-7
	O1 (B)	70		-207	82	-12

Table S18. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **j** with the selected radical species in methanol.

j		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-79	87	-165	-75	-3
	N2 (A)	-92		-179	-82	-11
	N2 (B)	-44		-131	-16	-28
	O1 (B)	-74		-161	-40	-34
$\cdot OC(CH_3)_3$	N1 (A)	-87	87	-174	-84	-3
	N2 (A)	-101		-188	-90	-10
	N2 (B)	-52		-139	-24	-28
	O1 (B)	-82		-169	-49	-33
$\cdot OH$	N1 (A)	-150	8	-158	-68	-82
	N2 (A)	-164		-172	-74	-90
	N2 (B)	-115		-123	-8	-107
	O1 (B)	-145		-153	-33	-112
$\cdot OOH$	N1 (A)	-10	109	-119	-29	19
	N2 (A)	-24		-133	-36	12
	N2 (B)	25		-85	30	-6
	O1 (B)	-5		-115	6	-11
$\cdot OOCH_3$	N1 (A)	-3	118	-121	-31	28
	N2 (A)	-17		-134	-37	20
	N2 (B)	32		-86	29	3
	O1 (B)	2		-116	4	-3
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-2	98	-101	-11	8
	N2 (A)	-16		-114	-17	1
	N2 (B)	32		-66	49	-16
	O1 (B)	2		-96	24	-22
DPPH	N1 (A)	26	86	-60	30	-4
	N2 (A)	12		-74	23	-11
	N2 (B)	61		-26	89	-28
	O1 (B)	31		-56	65	-34
$O_2^{\cdot -}$	N1 (A)	62	276	-214	43	19
	N2 (A)	48		-228	37	12
	N2 (B)	97		-179	102	-6
	O1 (B)	67		-209	78	-11

Table S19. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **k** with the selected radical species in methanol.

k		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-85	80	-165	-71	-14
	N2 (A)	-94		-174	-79	-15
	N2 (B)	-43		-123	-13	-30
	O1 (B)	-81		-161	-40	-41
$\cdot OC(CH_3)_3$	N1 (A)	-93	81	-174	-80	-13
	N2 (A)	-102		-183	-87	-15
	N2 (B)	-51		-132	-21	-30
	O1 (B)	-89		-169	-48	-40
$\cdot OH$	N1 (A)	-156	1	-158	-64	-93
	N2 (A)	-165		-167	-71	-94
	N2 (B)	-115		-116	-5	-109
	O1 (B)	-152		-153	-32	-120
$\cdot OOH$	N1 (A)	-16	103	-119	-25	9
	N2 (A)	-25		-128	-33	7
	N2 (B)	25		-77	33	-8
	O1 (B)	-12		-115	6	-18
$\cdot OOCH_3$	N1 (A)	-9	111	-120	-26	17
	N2 (A)	-18		-129	-34	16
	N2 (B)	33		-79	32	1
	O1 (B)	-5		-116	5	-10
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-9	92	-100	-6	-2
	N2 (A)	-18		-110	-14	-4
	N2 (B)	33		-59	52	-19
	O1 (B)	-4		-96	25	-29
DPPH	N1 (A)	20	80	-60	34	-14
	N2 (A)	11		-69	26	-16
	N2 (B)	61		-18	92	-31
	O1 (B)	24		-56	65	-41
$O_2^{\cdot -}$	N1 (A)	56	269	-214	47	9
	N2 (A)	47		-223	39	7
	N2 (B)	97		-172	105	-8
	O1 (B)	60		-209	78	-18

Table S20. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **l** with the selected radical species in methanol.

l		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-83	80	-163	-72	-11
	N2 (A)	-95		-175	-78	-18
	N2 (B)	-46		-126	-12	-34
	O1 (B)	-74		-154	-35	-39
$\cdot OC(CH_3)_3$	N1 (A)	-91	80	-171	-81	-11
	N2 (A)	-104		-184	-87	-17
	N2 (B)	-55		-135	-21	-34
	O1 (B)	-83		-163	-43	-39
$\cdot OH$	N1 (A)	-154	1	-155	-65	-90
	N2 (A)	-167		-168	-70	-96
	N2 (B)	-118		-119	-5	-113
	O1 (B)	-146		-147	-27	-118
$\cdot OOH$	N1 (A)	-14	102	-117	-26	11
	N2 (A)	-27		-129	-32	5
	N2 (B)	22		-80	34	-12
	O1 (B)	-6		-108	11	-17
$\cdot OOCH_3$	N1 (A)	-7	111	-118	-27	20
	N2 (A)	-20		-130	-33	14
	N2 (B)	30		-81	33	-3
	O1 (B)	1		-109	10	-8
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-7	91	-98	-7	0
	N2 (A)	-19		-110	-13	-6
	N2 (B)	30		-61	53	-23
	O1 (B)	2		-89	30	-28
DPPH	N1 (A)	22	79	-58	33	-12
	N2 (A)	9		-70	27	-18
	N2 (B)	58		-21	93	-35
	O1 (B)	30		-49	70	-40
$O_2^{\cdot -}$	N1 (A)	58	269	-211	46	11
	N2 (A)	45		-224	40	5
	N2 (B)	94		-174	106	-12
	O1 (B)	66		-202	83	-17

Table S21. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **n** with the selected radical species in methanol.

n		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	73	-153	-75	-5
	N2 (A)	-94		-168	-78	-16
	N2 (B)	-46		-120	-12	-35
	O1 (B)	-75		-148	-35	-40
	O2 (C)	-108		-181	-72	-36
	O3 (C)	-111		-184	-71	-40
$\cdot OC(CH_3)_3$	N1 (A)	-88	74	-162	-83	-5
	N2 (A)	-103		-176	-87	-16
	N2 (B)	-55		-128	-20	-34
	O1 (B)	-83		-156	-43	-40
	O2 (C)	-116		-190	-80	-36
	O3 (C)	-119		-193	-80	-39
$\cdot OH$	N1 (A)	-151	-6	-146	-67	-84
	N2 (A)	-166		-160	-71	-95
	N2 (B)	-118		-112	-4	-113
	O1 (B)	-146		-140	-27	-119
	O2 (C)	-179		-174	-64	-115
	O3 (C)	-182		-177	-63	-119
$\cdot OOH$	N1 (A)	-11	96	-107	-29	17
	N2 (A)	-26		-122	-32	6
	N2 (B)	22		-73	34	-12
	O1 (B)	-6		-102	12	-18
	O2 (C)	-39		-135	-26	-14
	O3 (C)	-42		-138	-25	-17
$\cdot OOCH_3$	N1 (A)	-4	104	-108	-30	26
	N2 (A)	-19		-123	-33	15
	N2 (B)	29		-75	33	-4
	O1 (B)	1		-103	10	-9
	O2 (C)	-22		-126	-12	-10
	O3 (C)	-35		-139	-26	-9
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	85	-88	-10	6
	N2 (A)	-18		-103	-13	-5
	N2 (B)	30		-55	53	-23
	O1 (B)	2		-83	30	-29
	O2 (C)	-32		-116	-7	-25
	O3 (C)	-34		-119	-6	-28
DPPH	N1 (A)	25	73	-48	30	-6
	N2 (A)	10		-63	27	-17
	N2 (B)	58		-15	93	-35
	O1 (B)	30		-43	70	-41
	O2 (C)	-3		-76	33	-37
	O3 (C)	-6		-79	34	-40
$O_2^{\cdot-}$	N1 (A)	61	262	-202	43	17
	N2 (A)	46		-216	40	6
	N2 (B)	94		-168	106	-12
	O1 (B)	33		-230	46	-14
	O2 (C)	43		-219	62	-19
	O3 (C)	30		-232	47	-17

Table S22. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **o** with the selected radical species in methanol.

o		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-79	77	-156	-73	-7
	N2 (A)	-94		-171	-78	-16
	N2 (B)	-46		-123	-12	-34
	O1 (B)	-78		-155	-42	-36
	O1 (C)	-100		-177	-56	-44
$\cdot OC(CH_3)_3$	N1 (A)	-88	77	-165	-81	-7
	N2 (A)	-103		-180	-87	-16
	N2 (B)	-55		-132	-21	-34
	O1 (B)	-86		-163	-50	-36
	O1 (C)	-109		-186	-65	-44
$\cdot OH$	N1 (A)	-151	-2	-149	-65	-86
	N2 (A)	-166		-164	-71	-95
	N2 (B)	-118		-116	-5	-113
	O1 (B)	-149		-147	-34	-115
	O1 (C)	-172		-170	-48	-123
$\cdot OOH$	N1 (A)	-11	99	-110	-26	15
	N2 (A)	-26		-125	-32	6
	N2 (B)	22		-77	34	-12
	O1 (B)	-9		-108	4	-14
	O1 (C)	-32		-131	-10	-22
$\cdot OOCH_3$	N1 (A)	-4	108	-111	-28	24
	N2 (A)	-19		-126	-34	15
	N2 (B)	29		-78	33	-3
	O1 (B)	-2		-110	3	-5
	O1 (C)	-25		-132	-11	-13
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-3	88	-91	-8	5
	N2 (A)	-18		-106	-14	-5
	N2 (B)	30		-58	53	-23
	O1 (B)	-2		-90	23	-25
	O1 (C)	-24		-112	9	-33
DPPH	N1 (A)	25	76	-51	33	-7
	N2 (A)	10		-66	27	-17
	N2 (B)	58		-18	93	-35
	O1 (B)	27		-49	63	-37
	O1 (C)	4		-72	49	-45
$O_2^{\cdot -}$	N1 (A)	61	266	-205	46	15
	N2 (A)	46		-220	40	6
	N2 (B)	94		-172	106	-12
	O1 (B)	63		-203	76	-14
	O1 (C)	40		-226	62	-22

Table S23. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **p** with the selected radical species in methanol.

p		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	67	-148	-72	-9
	N2 (A)	-96		-162	-78	-18
	N2 (B)	-47		-114	-13	-34
	O1 (B)	-74		-141	-35	-39
	O3 (C)	-103		-170	-55	-48
$\cdot OC(CH_3)_3$	N1 (A)	-89	67	-156	-81	-8
	N2 (A)	-104		-171	-87	-17
	N2 (B)	-55		-122	-21	-34
	O1 (B)	-82		-149	-44	-39
	O3 (C)	-112		-178	-63	-48
$\cdot OH$	N1 (A)	-153	-12	-140	-65	-88
	N2 (A)	-167		-155	-71	-96
	N2 (B)	-119		-106	-5	-113
	O1 (B)	-146		-133	-28	-118
	O3 (C)	-175		-162	-47	-127
$\cdot OOH$	N1 (A)	-13	89	-101	-26	14
	N2 (A)	-27		-116	-32	5
	N2 (B)	21		-67	33	-12
	O1 (B)	-6		-95	11	-17
	O3 (C)	-35		-124	-9	-26
$\cdot OOCH_3$	N1 (A)	-5	98	-103	-28	22
	N2 (A)	-20		-117	-33	14
	N2 (B)	29		-69	32	-3
	O1 (B)	2		-96	9	-8
	O3 (C)	-27		-125	-10	-17
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-5	78	-83	-8	3
	N2 (A)	-19		-97	-13	-6
	N2 (B)	29		-49	52	-23
	O1 (B)	2		-76	29	-27
	O3 (C)	-27		-105	10	-37
DPPH	N1 (A)	23	66	-43	33	-9
	N2 (A)	9		-57	27	-18
	N2 (B)	57		-9	92	-35
	O1 (B)	30		-36	70	-39
	O3 (C)	1		-65	50	-49
$O_2\cdot^-$	N1 (A)	59	256	-196	46	14
	N2 (A)	45		-211	40	5
	N2 (B)	93		-162	105	-12
	O1 (B)	66		-189	83	-17
	O3 (C)	37		-218	63	-26

Table S24. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **q** with the selected radical species in methanol.

q		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	60	-140	-72	-8
	N2 (A)	-95		-154	-78	-16
	N2 (B)	-46		-105	-12	-33
	O1 (B)	-74		-133	-33	-41
	O3 (C)	-119		-179	-55	-64
$\cdot OC(CH_3)_3$	N1 (A)	-88	60	-148	-81	-8
	N2 (A)	-103		-163	-87	-16
	N2 (B)	-54		-114	-21	-33
	O1 (B)	-82		-142	-42	-40
	O3 (C)	-127		-187	-64	-64
$\cdot OH$	N1 (A)	-151	-19	-132	-65	-87
	N2 (A)	-166		-147	-71	-95
	N2 (B)	-117		-98	-5	-112
	O1 (B)	-145		-126	-26	-120
	O3 (C)	-191		-171	-48	-143
$\cdot OOH$	N1 (A)	-11	82	-93	-26	14
	N2 (A)	-26		-108	-32	6
	N2 (B)	23		-59	34	-11
	O1 (B)	-5		-87	13	-18
	O3 (C)	-51		-133	-9	-42
$\cdot OOCH_3$	N1 (A)	-4	91	-95	-27	23
	N2 (A)	-19		-110	-34	15
	N2 (B)	30		-61	32	-2
	O1 (B)	2		-89	12	-10
	O3 (C)	-43		-134	-10	-33
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	71	-75	-7	4
	N2 (A)	-19		-90	-14	-5
	N2 (B)	30		-41	52	-22
	O1 (B)	2		-69	32	-29
	O3 (C)	-43		-114	10	-53
DPPH	N1 (A)	25	59	-35	33	-8
	N2 (A)	10		-49	27	-17
	N2 (B)	59		0	93	-34
	O1 (B)	31		-28	72	-41
	O3 (C)	-15		-74	50	-65
$O_2^{\cdot -}$	N1 (A)	61	249	-188	46	14
	N2 (A)	46		-203	40	6
	N2 (B)	95		-154	106	-11
	O1 (B)	67		-182	85	-18
	O3 (C)	21		-227	63	-42

Table S25. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **r** with the selected radical species in methanol.

r		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	82	-162	-72	-8
	N2 (A)	-94		-176	-78	-16
	N2 (B)	-46		-127	-13	-33
	O1 (B)	-74		-156	-36	-38
	O2 (C)	-92		-173	-65	-27
$\cdot OC(CH_3)_3$	N1 (A)	-88	82	-170	-81	-7
	N2 (A)	-103		-185	-87	-16
	N2 (B)	-54		-136	-22	-33
	O1 (B)	-82		-164	-45	-38
	O2 (C)	-100		-182	-74	-26
$\cdot OH$	N1 (A)	-152	3	-154	-65	-87
	N2 (A)	-166		-168	-71	-95
	N2 (B)	-117		-120	-6	-112
	O1 (B)	-145		-148	-29	-117
	O2 (C)	-163		-166	-58	-106
$\cdot OOH$	N1 (A)	-12	104	-116	-26	15
	N2 (A)	-26		-130	-32	6
	N2 (B)	23		-81	33	-10
	O1 (B)	-5		-109	10	-16
	O2 (C)	-23		-127	-19	-4
$\cdot OOCH_3$	N1 (A)	-4	113	-117	-28	23
	N2 (A)	-19		-131	-34	15
	N2 (B)	30		-83	32	-2
	O1 (B)	2		-111	9	-7
	O2 (C)	-16		-129	-20	4
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	93	-97	-8	4
	N2 (A)	-18		-111	-14	-5
	N2 (B)	30		-63	52	-21
	O1 (B)	2		-91	29	-26
	O2 (C)	-16		-109	0	-15
DPPH	N1 (A)	24	81	-57	33	-8
	N2 (A)	10		-71	27	-17
	N2 (B)	59		-22	92	-33
	O1 (B)	31		-50	69	-38
	O2 (C)	13		-68	40	-27
$O_2^{\cdot -}$	N1 (A)	60	270	-210	46	15
	N2 (A)	46		-224	40	6
	N2 (B)	95		-176	105	-10
	O1 (B)	67		-204	82	-16
	O2 (C)	49		-222	53	-4

Table S26. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **s** with the selected radical species in methanol.

s		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	62	-141	-73	-7
	N2 (A)	-95		-156	-79	-16
	N2 (B)	-46		-107	-13	-33
	O1 (B)	-74		-135	-35	-39
$\cdot OC(CH_3)_3$	N1 (A)	-88	62	-150	-81	-7
	N2 (A)	-103		-165	-87	-15
	N2 (B)	-54		-116	-21	-33
	O1 (B)	-82		-144	-44	-38
$\cdot OH$	N1 (A)	-151	-17	-134	-65	-86
	N2 (A)	-166		-149	-71	-95
	N2 (B)	-117		-100	-5	-112
	O1 (B)	-145		-128	-28	-117
$\cdot OOH$	N1 (A)	-11	84	-95	-26	15
	N2 (A)	-26		-110	-33	7
	N2 (B)	23		-61	33	-11
	O1 (B)	-5		-89	11	-16
$\cdot OOCH_3$	N1 (A)	-4	93	-97	-28	24
	N2 (A)	-19		-111	-34	15
	N2 (B)	30		-63	32	-2
	O1 (B)	2		-90	10	-7
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	73	-77	-8	4
	N2 (A)	-18		-91	-14	-4
	N2 (B)	30		-43	52	-22
	O1 (B)	3		-70	30	-27
DPPH	N1 (A)	25	61	-36	32	-8
	N2 (A)	10		-51	26	-16
	N2 (B)	59		-2	92	-34
	O1 (B)	31		-30	70	-39
$O_2^{\cdot -}$	N1 (A)	61	251	-190	46	15
	N2 (A)	46		-205	39	7
	N2 (B)	95		-156	105	-11
	O1 (B)	67		-184	83	-16

Table S27. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **t** with the selected radical species in methanol.

t		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-78	55	-132	-76	-2
	N2 (A)	-93		-147	-82	-11
	N2 (B)	-45		-100	-15	-30
	O1 (B)	-77		-131	-45	-32
	O1 (C)	-88		-142	-83	-4
$\cdot OC(CH_3)_3$	N1 (A)	-86	55	-141	-84	-2
	N2 (A)	-101		-156	-91	-11
	N2 (B)	-53		-108	-23	-30
	O1 (B)	-85		-140	-54	-31
	O1 (C)	-96		-151	-92	-4
$\cdot OH$	N1 (A)	-149	-24	-125	-68	-81
	N2 (A)	-164		-140	-74	-90
	N2 (B)	-117		-92	-7	-109
	O1 (B)	-148		-124	-38	-110
	O1 (C)	-159		-135	-76	-83
$\cdot OOH$	N1 (A)	-9	77	-86	-29	20
	N2 (A)	-24		-101	-36	11
	N2 (B)	23		-53	31	-8
	O1 (B)	-8		-85	1	-9
	O1 (C)	-19		-96	-37	18
$\cdot OOCH_3$	N1 (A)	-2	86	-88	-31	29
	N2 (A)	-17		-103	-37	20
	N2 (B)	31		-55	30	1
	O1 (B)	-1		-86	0	-1
	O1 (C)	-12		-97	-39	27
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-2	66	-68	-11	9
	N2 (A)	-17		-83	-17	1
	N2 (B)	31		-35	50	-19
	O1 (B)	0		-66	20	-20
	O1 (C)	-11		-77	-19	7
DPPH	N1 (A)	27	54	-27	30	-3
	N2 (A)	12		-42	23	-11
	N2 (B)	59		5	90	-31
	O1 (B)	28		-26	60	-32
	O1 (C)	17		-37	22	-5
$O_2^{\cdot -}$	N1 (A)	63	244	-181	43	20
	N2 (A)	48		-196	36	11
	N2 (B)	95		-148	103	-8
	O1 (B)	64		-180	73	-9
	O1 (C)	53		-191	35	18

Table S28. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **a** with the selected radical species in water.

a		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	73	-154	-72	-9
	N2 (A)	-95		-167	-76	-19
	N2 (B)	-46		-119	-13	-33
	O1 (B)	-73		-146	-35	-38
$\cdot OC(CH_3)_3$	N1 (A)	-90	73	-163	-81	-9
	N2 (A)	-104		-177	-85	-19
	N2 (B)	-55		-128	-22	-33
	O1 (B)	-82		-155	-45	-38
$\cdot OH$	N1 (A)	-151	-8	-144	-62	-90
	N2 (A)	-165		-157	-66	-99
	N2 (B)	-116		-109	-3	-113
	O1 (B)	-143		-135	-25	-118
$\cdot OOH$	N1 (A)	-14	93	-107	-25	11
	N2 (A)	-27		-120	-29	2
	N2 (B)	21		-72	34	-13
	O1 (B)	-5		-99	12	-17
$\cdot OOCH_3$	N1 (A)	-6	103	-109	-27	21
	N2 (A)	-20		-123	-31	11
	N2 (B)	29		-74	32	-3
	O1 (B)	2		-101	9	-8
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	81	-87	-5	-1
	N2 (A)	-20		-101	-9	-10
	N2 (B)	29		-52	54	-25
	O1 (B)	2		-79	32	-29
DPPH	N1 (A)	23	75	-52	30	-7
	N2 (A)	9		-66	26	-16
	N2 (B)	58		-17	89	-31
	O1 (B)	31		-44	67	-35
$O_2^{\cdot -}$	N1 (A)	57	248	-190	46	11
	N2 (A)	44		-204	42	2
	N2 (B)	92		-155	105	-13
	O1 (B)	66		-182	83	-17

Table S29. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **b** with the selected radical species in water.

b		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	71	-152	-73	-7
	N2 (A)	-96		-167	-78	-18
	N2 (B)	-47		-118	-14	-33
	O1 (B)	-77		-148	-42	-35
	O1 (C)	-81		-152	-57	-24
$\cdot OC(CH_3)_3$	N1 (A)	-89	71	-161	-82	-7
	N2 (A)	-105		-176	-87	-18
	N2 (B)	-56		-128	-23	-33
	O1 (B)	-86		-157	-51	-35
	O1 (C)	-90		-162	-67	-23
$\cdot OH$	N1 (A)	-150	-9	-141	-63	-88
	N2 (A)	-166		-157	-68	-98
	N2 (B)	-117		-108	-4	-113
	O1 (B)	-147		-138	-32	-115
	O1 (C)	-151		-142	-47	-104
$\cdot OOH$	N1 (A)	-13	92	-105	-26	13
	N2 (A)	-28		-120	-31	3
	N2 (B)	21		-71	33	-12
	O1 (B)	-9		-101	5	-14
	O1 (C)	-13		-105	-10	-3
$\cdot OOCH_3$	N1 (A)	-6	101	-107	-28	23
	N2 (A)	-21		-122	-33	12
	N2 (B)	28		-74	31	-3
	O1 (B)	-2		-103	3	-5
	O1 (C)	-6		-108	-13	7
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-5	80	-85	-6	1
	N2 (A)	-20		-100	-11	-10
	N2 (B)	28		-51	53	-25
	O1 (B)	-2		-81	25	-27
	O1 (C)	-6		-85	9	-15
DPPH	N1 (A)	24	74	-50	29	-5
	N2 (A)	9		-65	24	-16
	N2 (B)	57		-16	88	-31
	O1 (B)	28		-46	60	-33
	O1 (C)	23		-50	45	-21
$O_2^{\cdot -}$	N1 (A)	58	246	-188	45	13
	N2 (A)	43		-203	40	3
	N2 (B)	91		-155	104	-12
	O1 (B)	62		-184	76	-14
	O1 (C)	57		-189	61	-3

Table S30. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **c** with the selected radical species in water.

c		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	73	-155	-72	-9
	N2 (A)	-95		-168	-77	-18
	N2 (B)	-47		-120	-13	-34
	O1 (B)	-75		-148	-35	-40
	O2 (C)	-76		-149	-55	-21
$\cdot OC(CH_3)_3$	N1 (A)	-91	73	-164	-81	-9
	N2 (A)	-104		-178	-86	-18
	N2 (B)	-56		-129	-22	-33
	O1 (B)	-84		-157	-44	-39
	O2 (C)	-85		-158	-65	-20
$\cdot OH$	N1 (A)	-151	-7	-144	-62	-89
	N2 (A)	-165		-158	-67	-99
	N2 (B)	-117		-110	-3	-114
	O1 (B)	-145		-138	-25	-120
	O2 (C)	-146		-139	-45	-101
$\cdot OOH$	N1 (A)	-14	94	-108	-25	11
	N2 (A)	-28		-121	-30	2
	N2 (B)	21		-73	34	-13
	O1 (B)	-7		-101	12	-19
	O2 (C)	-8		-102	-8	0
$\cdot OOCH_3$	N1 (A)	-7	103	-110	-28	21
	N2 (A)	-20		-124	-32	12
	N2 (B)	28		-75	32	-3
	O1 (B)	0		-103	10	-9
	O2 (C)	-1		-104	-11	10
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	82	-88	-5	-1
	N2 (A)	-20		-102	-10	-10
	N2 (B)	29		-53	54	-25
	O1 (B)	1		-81	32	-31
	O2 (C)	-1		-82	12	-12
DPPH	N1 (A)	23	76	-53	30	-7
	N2 (A)	9		-67	25	-16
	N2 (B)	58		-18	89	-31
	O1 (B)	30		-46	67	-37
	O2 (C)	28		-47	47	-18
$O_2^{\cdot -}$	N1 (A)	57	248	-191	46	11
	N2 (A)	43		-205	41	2
	N2 (B)	92		-156	105	-13
	O1 (B)	64		-184	83	-19
	O2 (C)	63		-186	63	0

Table S31. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **d** with the selected radical species in water.

d		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	81	-163	-71	-10
	N2 (A)	-95		-176	-76	-19
	N2 (B)	-46		-127	-13	-33
	O1 (B)	-72		-154	-35	-38
	O4 (C)	-83		-164	-54	-29
$\cdot OC(CH_3)_3$	N1 (A)	-90	81	-172	-81	-10
	N2 (A)	-104		-186	-85	-19
	N2 (B)	-55		-137	-22	-33
	O1 (B)	-81		-163	-44	-37
	O4 (C)	-92		-174	-63	-29
$\cdot OH$	N1 (A)	-151	1	-152	-61	-90
	N2 (A)	-165		-166	-66	-99
	N2 (B)	-116		-117	-3	-113
	O1 (B)	-142		-143	-25	-118
	O4 (C)	-153		-154	-44	-109
$\cdot OOH$	N1 (A)	-14	102	-116	-24	11
	N2 (A)	-27		-129	-29	1
	N2 (B)	21		-80	34	-13
	O1 (B)	-5		-107	12	-17
	O4 (C)	-15		-117	-7	-8
$\cdot OOCH_3$	N1 (A)	-6	112	-118	-27	20
	N2 (A)	-20		-132	-31	11
	N2 (B)	29		-83	32	-3
	O1 (B)	3		-109	10	-7
	O4 (C)	-8		-120	-10	1
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	90	-96	-4	-2
	N2 (A)	-20		-109	-9	-11
	N2 (B)	29		-61	54	-25
	O1 (B)	3		-87	32	-29
	O4 (C)	-8		-97	13	-20
DPPH	N1 (A)	23	84	-61	31	-8
	N2 (A)	9		-74	26	-17
	N2 (B)	58		-25	89	-31
	O1 (B)	32		-52	67	-35
	O4 (C)	21		-62	48	-26
$O_2^{\cdot -}$	N1 (A)	57	256	-199	47	11
	N2 (A)	44		-213	42	1
	N2 (B)	92		-164	105	-13
	O1 (B)	66		-190	83	-17
	O4 (C)	56		-201	64	-8

Table S32. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **e** with the selected radical species in water.

e		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	75	-156	-74	-7
	N2 (A)	-94		-169	-78	-16
	N2 (B)	-46		-121	-15	-32
	O1 (B)	-73		-148	-36	-36
$\cdot OC(CH_3)_3$	N1 (A)	-90	75	-165	-83	-7
	N2 (A)	-103		-178	-87	-16
	N2 (B)	-55		-131	-24	-31
	O1 (B)	-82		-157	-46	-36
$\cdot OH$	N1 (A)	-151	-5	-146	-64	-87
	N2 (A)	-164		-159	-68	-96
	N2 (B)	-116		-111	-4	-112
	O1 (B)	-143		-137	-26	-116
$\cdot OOH$	N1 (A)	-13	96	-109	-27	14
	N2 (A)	-26		-122	-31	5
	N2 (B)	21		-74	32	-11
	O1 (B)	-5		-100	11	-16
$\cdot OOCH_3$	N1 (A)	-6	105	-111	-29	23
	N2 (A)	-19		-124	-33	14
	N2 (B)	29		-77	30	-1
	O1 (B)	2		-103	8	-6
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-5	83	-89	-7	1
	N2 (A)	-18		-102	-11	-7
	N2 (B)	29		-54	52	-23
	O1 (B)	3		-81	31	-28
DPPH	N1 (A)	24	77	-54	28	-5
	N2 (A)	11		-67	24	-13
	N2 (B)	58		-19	87	-29
	O1 (B)	32		-46	66	-34
$O_2^{\cdot -}$	N1 (A)	58	250	-192	44	14
	N2 (A)	45		-205	40	5
	N2 (B)	92		-158	103	-11
	O1 (B)	66		-184	82	-16

Table S33. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **f** with the selected radical species in water.

f		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	75	-155	-75	-5
	N2 (A)	-94		-169	-77	-17
	N2 (B)	-46		-120	-17	-29
	O1 (B)	-72		-147	-36	-36
$\cdot OC(CH_3)_3$	N1 (A)	-90	75	-165	-85	-5
	N2 (A)	-103		-178	-86	-16
	N2 (B)	-55		-130	-26	-29
	O1 (B)	-81		-156	-45	-36
$\cdot OH$	N1 (A)	-151	-5	-145	-65	-86
	N2 (A)	-164		-158	-67	-97
	N2 (B)	-116		-110	-7	-109
	O1 (B)	-142		-137	-26	-116
$\cdot OOH$	N1 (A)	-13	95	-108	-28	15
	N2 (A)	-26		-122	-30	4
	N2 (B)	22		-73	30	-8
	O1 (B)	-4		-100	11	-15
$\cdot OOCH_3$	N1 (A)	-6	105	-111	-31	25
	N2 (A)	-19		-124	-32	14
	N2 (B)	29		-76	28	2
	O1 (B)	3		-102	8	-6
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-5	83	-88	-8	3
	N2 (A)	-18		-102	-10	-8
	N2 (B)	30		-54	50	-20
	O1 (B)	3		-80	31	-28
DPPH	N1 (A)	24	77	-53	27	-3
	N2 (A)	11		-67	25	-14
	N2 (B)	59		-19	85	-26
	O1 (B)	32		-45	66	-34
$O_2^{\cdot -}$	N1 (A)	58	250	-192	43	15
	N2 (A)	45		-205	41	4
	N2 (B)	93		-157	101	-8
	O1 (B)	66		-183	82	-15

Table S34. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **g** with the selected radical species in water.

g		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	74	-155	-75	-6
	N2 (A)	-94		-168	-77	-17
	N2 (B)	-46		-120	-14	-32
	O1 (B)	-75		-149	-36	-39
$\cdot OC(CH_3)_3$	N1 (A)	-90	74	-164	-84	-6
	N2 (A)	-103		-178	-86	-17
	N2 (B)	-55		-129	-23	-32
	O1 (B)	-84		-158	-45	-39
$\cdot OH$	N1 (A)	-151	-6	-145	-65	-86
	N2 (A)	-164		-158	-67	-98
	N2 (B)	-116		-110	-4	-112
	O1 (B)	-145		-139	-26	-119
$\cdot OOH$	N1 (A)	-13	95	-108	-28	15
	N2 (A)	-27		-121	-30	3
	N2 (B)	22		-73	33	-11
	O1 (B)	-7		-102	11	-18
$\cdot OOCH_3$	N1 (A)	-6	104	-110	-30	24
	N2 (A)	-19		-124	-32	13
	N2 (B)	29		-75	31	-2
	O1 (B)	0		-104	9	-9
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	83	-88	-8	3
	N2 (A)	-19		-101	-10	-9
	N2 (B)	29		-53	53	-23
	O1 (B)	0		-82	31	-30
DPPH	N1 (A)	24	77	-53	27	-3
	N2 (A)	10		-66	25	-15
	N2 (B)	58		-18	88	-29
	O1 (B)	30		-47	66	-37
$O_2\cdot^-$	N1 (A)	58	249	-191	43	15
	N2 (A)	44		-205	41	3
	N2 (B)	93		-156	104	-11
	O1 (B)	64		-185	82	-18

Table S35. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **h** with the selected radical species in water.

h		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	79	-156	-75	-2
	N2 (A)	-89		-168	-80	-9
	N2 (B)	-42		-121	-15	-27
	O1 (B)	-73		-152	-42	-31
$\cdot OC(CH_3)_3$	N1 (A)	-85	80	-165	-84	-1
	N2 (A)	-98		-177	-89	-8
	N2 (B)	-51		-130	-24	-27
	O1 (B)	-82		-162	-51	-31
$\cdot OH$	N1 (A)	-146	-1	-145	-65	-82
	N2 (A)	-159		-158	-70	-89
	N2 (B)	-112		-111	-4	-107
	O1 (B)	-143		-142	-32	-111
$\cdot OOH$	N1 (A)	-9	100	-109	-28	19
	N2 (A)	-21		-121	-33	12
	N2 (B)	26		-74	32	-7
	O1 (B)	-5		-105	5	-11
$\cdot OOCH_3$	N1 (A)	-1	110	-111	-30	29
	N2 (A)	-14		-123	-35	22
	N2 (B)	33		-76	30	3
	O1 (B)	2		-108	3	-1
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	88	-89	-8	7
	N2 (A)	-13		-101	-13	0
	N2 (B)	34		-54	52	-19
	O1 (B)	2		-86	25	-23
DPPH	N1 (A)	28	82	-54	27	1
	N2 (A)	16		-66	22	-6
	N2 (B)	63		-19	87	-25
	O1 (B)	31		-51	60	-29
$O_2^{\cdot -}$	N1 (A)	62	254	-192	43	19
	N2 (A)	50		-204	38	12
	N2 (B)	97		-158	103	-7
	O1 (B)	65		-189	76	-11

Table S36. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **i** with the selected radical species in water.

i		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	77	-157	-74	-5
	N2 (A)	-93		-170	-79	-14
	N2 (B)	-45		-123	-15	-30
	O1 (B)	-71		-148	-37	-34
$\cdot OC(CH_3)_3$	N1 (A)	-89	77	-166	-84	-5
	N2 (A)	-102		-179	-88	-14
	N2 (B)	-55		-132	-25	-30
	O1 (B)	-80		-157	-47	-34
$\cdot OH$	N1 (A)	-150	-3	-147	-64	-85
	N2 (A)	-163		-160	-69	-94
	N2 (B)	-115		-112	-5	-110
	O1 (B)	-141		-138	-27	-114
$\cdot OOH$	N1 (A)	-12	98	-110	-27	15
	N2 (A)	-25		-123	-32	7
	N2 (B)	22		-75	32	-10
	O1 (B)	-3		-101	10	-13
$\cdot OOCH_3$	N1 (A)	-5	107	-112	-30	25
	N2 (A)	-18		-125	-34	16
	N2 (B)	29		-78	29	0
	O1 (B)	4		-104	7	-3
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	86	-90	-8	3
	N2 (A)	-17		-103	-12	-5
	N2 (B)	30		-56	52	-22
	O1 (B)	4		-81	30	-25
DPPH	N1 (A)	25	79	-55	27	-3
	N2 (A)	12		-68	23	-11
	N2 (B)	59		-21	87	-28
	O1 (B)	33		-46	65	-31
$O_2^{\cdot -}$	N1 (A)	59	252	-193	44	15
	N2 (A)	46		-206	39	7
	N2 (B)	93		-159	103	-10
	O1 (B)	68		-185	81	-13

Table S37. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **j** with the selected radical species in water.

j		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	78	-158	-75	-5
	N2 (A)	-92		-171	-79	-13
	N2 (B)	-44		-123	-16	-28
	O1 (B)	-72		-150	-39	-33
$\cdot OC(CH_3)_3$	N1 (A)	-89	79	-167	-84	-5
	N2 (A)	-101		-180	-88	-13
	N2 (B)	-53		-132	-25	-28
	O1 (B)	-81		-159	-49	-32
$\cdot OH$	N1 (A)	-150	-2	-148	-65	-85
	N2 (A)	-162		-160	-69	-93
	N2 (B)	-114		-113	-6	-108
	O1 (B)	-142		-140	-29	-113
$\cdot OOH$	N1 (A)	-12	99	-111	-28	16
	N2 (A)	-25		-124	-32	7
	N2 (B)	23		-76	31	-8
	O1 (B)	-4		-103	8	-12
$\cdot OOCH_3$	N1 (A)	-5	109	-113	-30	25
	N2 (A)	-17		-126	-34	17
	N2 (B)	31		-78	28	2
	O1 (B)	3		-106	5	-2
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	87	-91	-8	4
	N2 (A)	-17		-104	-12	-5
	N2 (B)	31		-56	51	-20
	O1 (B)	4		-83	28	-24
DPPH	N1 (A)	25	81	-56	27	-2
	N2 (A)	12		-69	23	-11
	N2 (B)	60		-21	86	-26
	O1 (B)	33		-48	63	-30
$O_2^{\cdot -}$	N1 (A)	59	253	-194	43	16
	N2 (A)	46		-207	39	7
	N2 (B)	94		-159	102	-8
	O1 (B)	67		-187	79	-12

Table S38. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **k** with the selected radical species in water.

k		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-79	75	-154	-69	-10
	N2 (A)	-92		-166	-74	-18
	N2 (B)	-42		-116	-12	-30
	O1 (B)	-75		-150	-37	-39
$\cdot OC(CH_3)_3$	N1 (A)	-88	75	-163	-79	-9
	N2 (A)	-101		-175	-83	-17
	N2 (B)	-51		-125	-21	-30
	O1 (B)	-84		-159	-46	-38
$\cdot OH$	N1 (A)	-149	-6	-143	-59	-90
	N2 (A)	-162		-156	-64	-98
	N2 (B)	-112		-106	-1	-110
	O1 (B)	-145		-140	-27	-119
$\cdot OOH$	N1 (A)	-11	95	-106	-22	11
	N2 (A)	-24		-119	-27	3
	N2 (B)	26		-69	36	-9
	O1 (B)	-8		-103	10	-18
$\cdot OOCH_3$	N1 (A)	-4	105	-109	-25	21
	N2 (A)	-17		-122	-29	13
	N2 (B)	33		-72	33	0
	O1 (B)	0		-105	8	-8
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	83	-87	-2	-1
	N2 (A)	-16		-99	-7	-9
	N2 (B)	34		-49	55	-22
	O1 (B)	0		-83	30	-30
DPPH	N1 (A)	25	77	-52	33	-7
	N2 (A)	13		-64	28	-15
	N2 (B)	63		-14	90	-28
	O1 (B)	29		-48	65	-36
$O_2^{\cdot -}$	N1 (A)	60	250	-190	49	11
	N2 (A)	47		-203	44	3
	N2 (B)	97		-153	107	-9
	O1 (B)	63		-186	81	-18

Table S39. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **l** with the selected radical species in water.

l		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-79	74	-153	-69	-10
	N2 (A)	-93		-168	-74	-19
	N2 (B)	-44		-119	-10	-34
	O1 (B)	-70		-144	-32	-38
$\cdot OC(CH_3)_3$	N1 (A)	-88	75	-162	-79	-9
	N2 (A)	-102		-177	-83	-19
	N2 (B)	-53		-128	-20	-34
	O1 (B)	-79		-154	-42	-37
$\cdot OH$	N1 (A)	-149	-6	-143	-59	-90
	N2 (A)	-163		-157	-64	-100
	N2 (B)	-114		-108	0	-114
	O1 (B)	-140		-134	-22	-118
$\cdot OOH$	N1 (A)	-11	95	-106	-22	11
	N2 (A)	-26		-120	-27	1
	N2 (B)	23		-72	37	-13
	O1 (B)	-2		-97	15	-17
$\cdot OOCH_3$	N1 (A)	-4	105	-109	-25	21
	N2 (A)	-18		-123	-29	11
	N2 (B)	31		-74	34	-4
	O1 (B)	5		-100	12	-7
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	83	-86	-2	-1
	N2 (A)	-18		-101	-7	-11
	N2 (B)	31		-52	56	-26
	O1 (B)	5		-77	35	-29
DPPH	N1 (A)	25	77	-51	33	-7
	N2 (A)	11		-66	28	-17
	N2 (B)	60		-17	92	-32
	O1 (B)	34		-42	70	-35
$O_2^{\cdot -}$	N1 (A)	60	249	-190	49	11
	N2 (A)	45		-204	44	1
	N2 (B)	94		-155	108	-13
	O1 (B)	69		-181	86	-17

Table S40. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **m** with the selected radical species in water.

m		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-80	76	-156	-72	-8
	N2 (A)	-93		-169	-77	-15
	N2 (B)	-46		-122	-13	-32
	O1 (B)	-78		-154	-38	-39
	O1 (C)	-108		-185	-73	-35
	O2 (C)	-104		-181	-72	-32
$\cdot OC(CH_3)_3$	N1 (A)	-89	77	-166	-81	-8
	N2 (A)	-102		-179	-87	-15
	N2 (B)	-55		-132	-23	-32
	O1 (B)	-87		-163	-47	-39
	O1 (C)	-117		-194	-82	-35
	O2 (C)	-113		-190	-81	-32
$\cdot OH$	N1 (A)	-150	-4	-146	-61	-88
	N2 (A)	-163		-159	-67	-96
	N2 (B)	-116		-112	-3	-113
	O1 (B)	-148		-144	-28	-120
	O1 (C)	-178		-174	-62	-116
	O2 (C)	-174		-170	-62	-112
$\cdot OOH$	N1 (A)	-12	97	-109	-25	12
	N2 (A)	-25		-122	-30	5
	N2 (B)	22		-75	34	-12
	O1 (B)	-10		-107	9	-19
	O1 (C)	-40		-137	-26	-15
	O2 (C)	-36		-133	-25	-11
$\cdot OOCH_3$	N1 (A)	-5	107	-112	-27	22
	N2 (A)	-18		-125	-33	15
	N2 (B)	29		-78	31	-2
	O1 (B)	-3		-109	6	-9
	O1 (C)	-33		-140	-28	-5
	O2 (C)	-29		-136	-27	-2
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-5	85	-89	-5	0
	N2 (A)	-17		-102	-11	-7
	N2 (B)	30		-55	53	-24
	O1 (B)	-2		-87	29	-31
	O1 (C)	-33		-118	-6	-27
	O2 (C)	-29		-114	-5	-24
DPPH	N1 (A)	24	79	-54	30	-6
	N2 (A)	12		-67	24	-13
	N2 (B)	59		-20	89	-30
	O1 (B)	27		-52	64	-37
	O1 (C)	-4		-83	29	-33
	O2 (C)	0		-79	30	-30
$O_2^{\cdot-}$	N1 (A)	59	251	-193	46	12
	N2 (A)	46		-206	41	5
	N2 (B)	93		-159	105	-12
	O1 (B)	61		-191	80	-19
	O1 (C)	31		-221	45	-15
	O2 (C)	34		-217	46	-11

Table S41. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **n** with the selected radical species in water.

n		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	66	-147	-72	-9
	N2 (A)	-95		-161	-76	-18
	N2 (B)	-47		-113	-13	-34
	O1 (B)	-73		-139	-35	-38
	O2 (C)	-109		-175	-70	-38
	O3 (C)	-109		-175	-70	-39
$\cdot OC(CH_3)_3$	N1 (A)	-90	67	-157	-81	-9
	N2 (A)	-104		-170	-86	-18
	N2 (B)	-56		-123	-22	-33
	O1 (B)	-82		-148	-44	-38
	O2 (C)	-118		-184	-80	-38
	O3 (C)	-118		-185	-79	-39
$\cdot OH$	N1 (A)	-151	-14	-137	-62	-89
	N2 (A)	-165		-151	-66	-98
	N2 (B)	-117		-103	-3	-114
	O1 (B)	-143		-129	-24	-118
	O2 (C)	-179		-165	-60	-118
	O3 (C)	-179		-165	-59	-119
$\cdot OOH$	N1 (A)	-13	87	-100	-25	11
	N2 (A)	-27		-114	-29	2
	N2 (B)	21		-66	34	-13
	O1 (B)	-5		-92	12	-17
	O2 (C)	-41		-128	-23	-18
	O3 (C)	-41		-128	-22	-19
$\cdot OOCH_3$	N1 (A)	-6	97	-103	-27	21
	N2 (A)	-20		-116	-32	12
	N2 (B)	28		-69	31	-3
	O1 (B)	2		-94	10	-8
	O2 (C)	-34		-130	-26	-8
	O3 (C)	-34		-131	-25	-9
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	75	-81	-5	-1
	N2 (A)	-19		-94	-10	-10
	N2 (B)	28		-47	54	-25
	O1 (B)	3		-72	32	-30
	O2 (C)	-33		-108	-3	-30
	O3 (C)	-33		-108	-3	-31
DPPH	N1 (A)	23	69	-46	30	-7
	N2 (A)	10		-59	25	-16
	N2 (B)	57		-11	89	-31
	O1 (B)	32		-37	67	-36
	O2 (C)	-4		-73	32	-36
	O3 (C)	-4		-73	32	-37
$O_2^{\cdot-}$	N1 (A)	58	242	-184	46	11
	N2 (A)	44		-198	42	2
	N2 (B)	92		-150	105	-13
	O1 (B)	66		-176	83	-17
	O2 (C)	30		-211	48	-18
	O3 (C)	30		-212	49	-19

Table S42. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **o** with the selected radical species in water.

o		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	69	-150	-73	-8
	N2 (A)	-97		-166	-77	-20
	N2 (B)	-47		-116	-14	-33
	O1 (B)	-76		-146	-41	-35
	O1 (C)	-99		-168	-54	-44
$\cdot OC(CH_3)_3$	N1 (A)	-90	70	-159	-82	-8
	N2 (A)	-106		-176	-87	-19
	N2 (B)	-56		-125	-23	-33
	O1 (B)	-85		-155	-51	-35
	O1 (C)	-108		-177	-64	-44
$\cdot OH$	N1 (A)	-151	-11	-140	-62	-88
	N2 (A)	-167		-156	-67	-100
	N2 (B)	-117		-106	-3	-113
	O1 (B)	-146		-136	-31	-115
	O1 (C)	-169		-158	-44	-125
$\cdot OOH$	N1 (A)	-13	90	-103	-26	13
	N2 (A)	-29		-119	-30	1
	N2 (B)	21		-69	33	-13
	O1 (B)	-9		-99	6	-15
	O1 (C)	-31		-121	-7	-24
$\cdot OOCH_3$	N1 (A)	-6	100	-105	-28	22
	N2 (A)	-22		-122	-33	11
	N2 (B)	28		-72	31	-3
	O1 (B)	-2		-101	3	-5
	O1 (C)	-24		-123	-10	-14
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-5	78	-83	-6	1
	N2 (A)	-22		-99	-10	-11
	N2 (B)	28		-49	53	-25
	O1 (B)	-1		-79	26	-27
	O1 (C)	-24		-101	13	-36
DPPH	N1 (A)	24	72	-48	29	-6
	N2 (A)	7		-64	25	-17
	N2 (B)	57		-14	88	-31
	O1 (B)	28		-44	61	-33
	O1 (C)	6		-66	48	-42
$O_2^{\cdot -}$	N1 (A)	58	244	-186	45	13
	N2 (A)	41		-203	41	1
	N2 (B)	92		-153	104	-13
	O1 (B)	62		-182	77	-15
	O1 (C)	40		-205	64	-24

Table S43. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **p** with the selected radical species in water.

p		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-82	59	-141	-72	-10
	N2 (A)	-96		-155	-76	-19
	N2 (B)	-48		-107	-14	-34
	O1 (B)	-73		-132	-35	-38
	O3 (C)	-102		-161	-54	-48
$\cdot OC(CH_3)_3$	N1 (A)	-91	60	-151	-82	-10
	N2 (A)	-105		-164	-86	-19
	N2 (B)	-57		-116	-23	-34
	O1 (B)	-82		-141	-44	-38
	O3 (C)	-111		-170	-63	-47
$\cdot OH$	N1 (A)	-152	-21	-131	-62	-90
	N2 (A)	-166		-145	-66	-99
	N2 (B)	-118		-97	-3	-114
	O1 (B)	-142		-122	-24	-118
	O3 (C)	-172		-151	-44	-128
$\cdot OOH$	N1 (A)	-14	80	-94	-25	11
	N2 (A)	-28		-108	-29	1
	N2 (B)	20		-60	34	-14
	O1 (B)	-5		-85	13	-17
	O3 (C)	-34		-114	-7	-27
$\cdot OOCH_3$	N1 (A)	-7	90	-97	-28	20
	N2 (A)	-21		-110	-32	11
	N2 (B)	27		-63	31	-4
	O1 (B)	2		-87	10	-8
	O3 (C)	-27		-116	-9	-17
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-7	68	-75	-5	-1
	N2 (A)	-20		-88	-9	-11
	N2 (B)	28		-40	53	-26
	O1 (B)	3		-65	32	-30
	O3 (C)	-26		-94	13	-39
DPPH	N1 (A)	22	62	-40	30	-7
	N2 (A)	9		-53	26	-17
	N2 (B)	57		-5	88	-32
	O1 (B)	32		-30	67	-36
	O3 (C)	3		-59	48	-45
$O_2^{\cdot -}$	N1 (A)	56	234	-178	46	11
	N2 (A)	43		-191	42	1
	N2 (B)	91		-144	104	-14
	O1 (B)	66		-168	83	-17
	O3 (C)	37		-197	64	-27

Table S44. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **q** with the selected radical species in water.

q		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	54	-135	-72	-9
	N2 (A)	-95		-148	-76	-19
	N2 (B)	-46		-100	-13	-33
	O1 (B)	-72		-126	-32	-40
	O3 (C)	-117		-171	-54	-63
$\cdot OC(CH_3)_3$	N1 (A)	-90	54	-144	-81	-9
	N2 (A)	-104		-158	-85	-18
	N2 (B)	-55		-109	-22	-33
	O1 (B)	-81		-135	-41	-40
	O3 (C)	-126		-180	-63	-63
$\cdot OH$	N1 (A)	-151	-26	-125	-62	-89
	N2 (A)	-165		-138	-66	-99
	N2 (B)	-116		-90	-3	-113
	O1 (B)	-142		-115	-22	-120
	O3 (C)	-187		-161	-44	-143
$\cdot OOH$	N1 (A)	-13	74	-88	-25	11
	N2 (A)	-27		-101	-29	2
	N2 (B)	22		-53	34	-13
	O1 (B)	-4		-79	15	-19
	O3 (C)	-50		-124	-7	-42
$\cdot OOCH_3$	N1 (A)	-6	84	-90	-27	21
	N2 (A)	-20		-104	-31	12
	N2 (B)	29		-55	32	-3
	O1 (B)	3		-81	13	-10
	O3 (C)	-42		-126	-10	-33
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	62	-68	-5	-1
	N2 (A)	-19		-82	-9	-10
	N2 (B)	29		-33	54	-25
	O1 (B)	4		-59	35	-31
	O3 (C)	-42		-104	13	-55
DPPH	N1 (A)	23	56	-33	30	-7
	N2 (A)	10		-46	26	-16
	N2 (B)	58		2	89	-31
	O1 (B)	33		-24	70	-37
	O3 (C)	-13		-69	48	-61
$O_2^{\cdot -}$	N1 (A)	58	229	-171	46	11
	N2 (A)	44		-185	42	2
	N2 (B)	92		-136	105	-13
	O1 (B)	67		-162	86	-19
	O3 (C)	21		-208	64	-42

Table S45. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **r** with the selected radical species in water.

r		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	73	-155	-75	-7
	N2 (A)	-94		-168	-77	-18
	N2 (B)	-46		-120	-14	-32
	O1 (B)	-72		-145	-35	-37
	O2 (C)	-90		-163	-64	-26
$\cdot OC(CH_3)_3$	N1 (A)	-90	74	-164	-84	-7
	N2 (A)	-103		-177	-86	-17
	N2 (B)	-55		-129	-23	-32
	O1 (B)	-81		-155	-45	-36
	O2 (C)	-99		-172	-73	-26
$\cdot OH$	N1 (A)	-151	-7	-145	-64	-87
	N2 (A)	-164		-158	-67	-98
	N2 (B)	-116		-110	-4	-113
	O1 (B)	-142		-135	-25	-117
	O2 (C)	-160		-153	-54	-106
$\cdot OOH$	N1 (A)	-14	94	-108	-28	14
	N2 (A)	-27		-121	-30	3
	N2 (B)	21		-73	33	-12
	O1 (B)	-4		-98	12	-16
	O2 (C)	-22		-116	-17	-5
$\cdot OOCH_3$	N1 (A)	-6	104	-110	-30	24
	N2 (A)	-19		-123	-32	13
	N2 (B)	28		-75	31	-2
	O1 (B)	3		-101	9	-6
	O2 (C)	-15		-119	-19	4
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	82	-88	-8	2
	N2 (A)	-19		-101	-10	-9
	N2 (B)	29		-53	53	-24
	O1 (B)	3		-79	32	-28
	O2 (C)	-14		-96	3	-17
DPPH	N1 (A)	23	76	-53	27	-4
	N2 (A)	10		-66	25	-15
	N2 (B)	58		-18	88	-30
	O1 (B)	32		-43	67	-34
	O2 (C)	15		-61	38	-23
$O_2^{\cdot -}$	N1 (A)	57	248	-191	43	14
	N2 (A)	44		-204	41	3
	N2 (B)	92		-156	104	-12
	O1 (B)	67		-182	83	-16
	O2 (C)	49		-200	54	-5

Table S46. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **s** with the selected radical species in water.

s		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-81	56	-136	-72	-8
	N2 (A)	-95		-150	-77	-18
	N2 (B)	-47		-102	-14	-33
	O1 (B)	-72		-128	-35	-37
$\cdot OC(CH_3)_3$	N1 (A)	-90	56	-146	-82	-8
	N2 (A)	-104		-159	-86	-17
	N2 (B)	-56		-111	-23	-33
	O1 (B)	-81		-137	-44	-37
$\cdot OH$	N1 (A)	-151	-25	-126	-62	-89
	N2 (A)	-165		-140	-67	-98
	N2 (B)	-117		-92	-4	-113
	O1 (B)	-142		-117	-25	-117
$\cdot OOH$	N1 (A)	-13	76	-89	-25	12
	N2 (A)	-27		-103	-30	3
	N2 (B)	21		-55	33	-12
	O1 (B)	-4		-80	12	-17
$\cdot OOCH_3$	N1 (A)	-6	86	-92	-28	22
	N2 (A)	-20		-105	-32	13
	N2 (B)	28		-58	31	-3
	O1 (B)	3		-83	10	-7
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-6	64	-70	-6	0
	N2 (A)	-19		-83	-10	-9
	N2 (B)	29		-35	53	-24
	O1 (B)	3		-61	32	-29
DPPH	N1 (A)	23	58	-35	30	-6
	N2 (A)	10		-48	25	-15
	N2 (B)	58		0	88	-30
	O1 (B)	32		-26	67	-35
$O_2^{\cdot -}$	N1 (A)	58	231	-173	46	12
	N2 (A)	44		-187	41	3
	N2 (B)	92		-139	104	-12
	O1 (B)	67		-164	83	-17

Table S47. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **t** with the selected radical species in water.

t		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-79	48	-127	-75	-4
	N2 (A)	-93		-141	-80	-13
	N2 (B)	-45		-93	-16	-30
	O1 (B)	-75		-123	-44	-31
	O1 (C)	-86		-133	-80	-6
$\cdot OC(CH_3)_3$	N1 (A)	-88	48	-137	-85	-4
	N2 (A)	-102		-150	-89	-13
	N2 (B)	-55		-103	-25	-29
	O1 (B)	-84		-132	-53	-31
	O1 (C)	-95		-143	-89	-5
$\cdot OH$	N1 (A)	-149	-32	-117	-65	-84
	N2 (A)	-163		-131	-70	-93
	N2 (B)	-115		-83	-6	-110
	O1 (B)	-145		-113	-34	-111
	O1 (C)	-156		-123	-70	-86
$\cdot OOH$	N1 (A)	-12	68	-80	-28	16
	N2 (A)	-25		-94	-33	7
	N2 (B)	22		-46	31	-9
	O1 (B)	-8		-76	3	-10
	O1 (C)	-18		-86	-33	15
$\cdot OOCH_3$	N1 (A)	-4	78	-83	-31	26
	N2 (A)	-18		-96	-35	17
	N2 (B)	29		-49	29	1
	O1 (B)	0		-78	1	-1
	O1 (C)	-11		-89	-35	25
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-4	56	-60	-8	4
	N2 (A)	-18		-74	-13	-5
	N2 (B)	30		-26	51	-21
	O1 (B)	0		-56	23	-23
	O1 (C)	-10		-67	-13	3
DPPH	N1 (A)	25	50	-25	27	-2
	N2 (A)	11		-39	22	-11
	N2 (B)	59		9	86	-27
	O1 (B)	29		-21	58	-29
	O1 (C)	19		-31	22	-3
$O_2\cdot^-$	N1 (A)	59	223	-164	43	16
	N2 (A)	45		-177	38	7
	N2 (B)	93		-130	102	-9
	O1 (B)	63		-160	74	-10
	O1 (C)	53		-170	38	15

Table S48. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **a** with the selected radical species in benzene.

a		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	283	-359	-144	68
	N2 (A)	-103		-386	-173	70
	N2 (B)	-36		-319	-74	38
	O1 (B)	-72		-355	-42	-31
$\cdot OC(CH_3)_3$	N1 (A)	-85	271	-356	-141	56
	N2 (A)	-113		-383	-171	58
	N2 (B)	-45		-316	-71	25
	O1 (B)	-81		-352	-39	-43
$\cdot OH$	N1 (A)	-145	235	-379	-165	20
	N2 (A)	-172		-407	-194	22
	N2 (B)	-105		-340	-95	-10
	O1 (B)	-141		-376	-63	-79
$\cdot OOH$	N1 (A)	-8	319	-327	-113	105
	N2 (A)	-35		-355	-142	107
	N2 (B)	32		-288	-43	74
	O1 (B)	-4		-324	-10	6
$\cdot OOCH_3$	N1 (A)	1	323	-322	-107	108
	N2 (A)	-27		-350	-137	110
	N2 (B)	40		-282	-37	78
	O1 (B)	5		-318	-5	10
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	275	-275	-61	60
	N2 (A)	-28		-303	-90	62
	N2 (B)	39		-236	9	29
	O1 (B)	3		-272	42	-39
DPPH	N1 (A)	20	176	-156	59	-39
	N2 (A)	-8		-184	29	-37
	N2 (B)	59		-117	129	-70
	O1 (B)	23		-152	161	-138
$O_2^{\cdot -}$	N1 (A)	88	806	-717	-17	105
	N2 (A)	61		-745	-46	107
	N2 (B)	128		-678	54	74
	O1 (B)	92		-714	86	6

Table S49. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **b** with the selected radical species in benzene.

b		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-75	276	-351	-142	67
	N2 (A)	-103		-379	-168	65
	N2 (B)	-38		-313	-70	32
	O1 (B)	-76		-351	-87	11
	O1 (C)	-81		-357	-129	48
$\cdot OC(CH_3)_3$	N1 (A)	-84	263	-348	-139	55
	N2 (A)	-112		-376	-165	53
	N2 (B)	-47		-310	-67	20
	O1 (B)	-85		-348	-84	-1
	O1 (C)	-91		-354	-126	36
$\cdot OH$	N1 (A)	-144	227	-371	-163	19
	N2 (A)	-172		-400	-189	17
	N2 (B)	-107		-334	-91	-16
	O1 (B)	-145		-372	-107	-37
	O1 (C)	-150		-378	-150	0
$\cdot OOH$	N1 (A)	-7	312	-319	-110	103
	N2 (A)	-35		-347	-137	102
	N2 (B)	30		-282	-39	69
	O1 (B)	-8		-320	-55	47
	O1 (C)	-14		-326	-98	84
$\cdot OOCH_3$	N1 (A)	2	316	-314	-105	107
	N2 (A)	-26		-342	-132	105
	N2 (B)	39		-277	-33	72
	O1 (B)	1		-314	-50	51
	O1 (C)	-5		-320	-93	88
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	267	-267	-59	59
	N2 (A)	-28		-295	-85	57
	N2 (B)	37		-230	13	24
	O1 (B)	-1		-268	-3	3
	O1 (C)	-6		-274	-46	40
DPPH	N1 (A)	21	168	-148	61	-40
	N2 (A)	-8		-176	34	-42
	N2 (B)	58		-111	132	-75
	O1 (B)	20		-149	116	-96
	O1 (C)	14		-154	73	-59
$O_2^{\cdot -}$	N1 (A)	89	799	-709	-14	103
	N2 (A)	61		-738	-41	102
	N2 (B)	126		-672	57	69
	O1 (B)	88		-710	41	47
	O1 (C)	83		-716	-2	84

Table S50. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **c** with the selected radical species in benzene.

c		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	281	-357	-144	68
	N2 (A)	-104		-385	-173	69
	N2 (B)	-37		-317	-72	35
	O1 (B)	-73		-354	-91	18
	O2 (C)	-69		-350	-105	36
$\cdot OC(CH_3)_3$	N1 (A)	-85	269	-354	-141	56
	N2 (A)	-113		-382	-170	57
	N2 (B)	-46		-314	-69	23
	O1 (B)	-82		-351	-88	6
	O2 (C)	-78		-347	-102	24
$\cdot OH$	N1 (A)	-145	233	-378	-165	20
	N2 (A)	-173		-405	-194	21
	N2 (B)	-106		-338	-93	-13
	O1 (B)	-142		-375	-112	-30
	O2 (C)	-138		-371	-126	-12
$\cdot OOH$	N1 (A)	-8	317	-325	-112	104
	N2 (A)	-36		-353	-142	106
	N2 (B)	31		-286	-41	72
	O1 (B)	-5		-322	-60	54
	O2 (C)	-1		-318	-74	73
$\cdot OOCH_3$	N1 (A)	1	321	-320	-107	108
	N2 (A)	-27		-348	-137	109
	N2 (B)	40		-281	-35	75
	O1 (B)	4		-317	-54	58
	O2 (C)	8		-313	-69	76
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	273	-273	-60	60
	N2 (A)	-29		-301	-90	61
	N2 (B)	39		-234	11	27
	O1 (B)	2		-271	-8	10
	O2 (C)	6		-266	-22	28
DPPH	N1 (A)	20	174	-154	59	-39
	N2 (A)	-8		-182	29	-38
	N2 (B)	59		-115	131	-72
	O1 (B)	22		-151	112	-89
	O2 (C)	27		-147	97	-71
$O_2^{\cdot -}$	N1 (A)	88	804	-715	-16	104
	N2 (A)	60		-743	-46	106
	N2 (B)	127		-676	56	72
	O1 (B)	91		-713	37	54
	O2 (C)	95		-709	22	73

Table S51. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **d** with the selected radical species in benzene.

d		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	282	-358	-143	68
	N2 (A)	-104		-386	-172	69
	N2 (B)	-37		-319	-74	38
	O1 (B)	-71		-353	-42	-30
	O3 (C)	-76		-358	-101	25
$\cdot OC(CH_3)_3$	N1 (A)	-85	270	-355	-140	55
	N2 (A)	-113		-383	-169	57
	N2 (B)	-46		-316	-71	25
	O1 (B)	-80		-350	-39	-42
	O3 (C)	-85		-355	-98	13
$\cdot OH$	N1 (A)	-145	234	-379	-164	20
	N2 (A)	-173		-407	-193	21
	N2 (B)	-106		-340	-95	-11
	O1 (B)	-140		-374	-63	-78
	O3 (C)	-145		-379	-122	-23
$\cdot OOH$	N1 (A)	-8	319	-327	-112	104
	N2 (A)	-36		-354	-141	105
	N2 (B)	31		-288	-43	74
	O1 (B)	-3		-322	-10	7
	O3 (C)	-8		-326	-70	62
$\cdot OOCH_3$	N1 (A)	1	322	-321	-107	108
	N2 (A)	-27		-349	-136	109
	N2 (B)	40		-282	-38	78
	O1 (B)	6		-317	-5	10
	O3 (C)	1		-321	-64	65
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	274	-275	-60	60
	N2 (A)	-28		-303	-89	61
	N2 (B)	38		-236	9	29
	O1 (B)	4		-270	42	-38
	O3 (C)	0		-274	-18	17
DPPH	N1 (A)	20	175	-155	59	-39
	N2 (A)	-8		-183	30	-38
	N2 (B)	59		-116	128	-70
	O1 (B)	24		-151	161	-137
	O3 (C)	20		-155	102	-82
$O_2\cdot^-$	N1 (A)	88	805	-717	-16	104
	N2 (A)	60		-745	-45	105
	N2 (B)	127		-678	53	74
	O1 (B)	93		-712	86	7
	O3 (C)	89		-717	27	62

Table S52. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **e** with the selected radical species in benzene.

e		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-74	289	-363	-149	75
	N2 (A)	-101		-390	-178	77
	N2 (B)	-35		-324	-79	44
	O1 (B)	-70		-359	-49	-22
$\cdot OC(CH_3)_3$	N1 (A)	-83	277	-360	-146	63
	N2 (A)	-111		-387	-176	65
	N2 (B)	-45		-321	-76	32
	O1 (B)	-80		-356	-46	-34
$\cdot OH$	N1 (A)	-143	241	-384	-170	27
	N2 (A)	-170		-411	-199	29
	N2 (B)	-104		-345	-100	-4
	O1 (B)	-139		-380	-70	-70
$\cdot OOH$	N1 (A)	-6	325	-332	-118	112
	N2 (A)	-34		-359	-147	114
	N2 (B)	33		-293	-48	81
	O1 (B)	-2		-328	-17	15
$\cdot OOCH_3$	N1 (A)	3	329	-326	-112	115
	N2 (A)	-25		-353	-142	117
	N2 (B)	41		-287	-43	84
	O1 (B)	6		-322	-12	18
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	1	281	-280	-66	67
	N2 (A)	-26		-307	-95	69
	N2 (B)	40		-241	4	36
	O1 (B)	5		-276	34	-30
DPPH	N1 (A)	21	182	-160	53	-32
	N2 (A)	-6		-187	24	-30
	N2 (B)	60		-121	123	-63
	O1 (B)	25		-156	154	-129
$O_2^{\cdot -}$	N1 (A)	90	812	-722	-22	112
	N2 (A)	63		-749	-51	114
	N2 (B)	129		-683	48	81
	O1 (B)	94		-718	79	15

Table S53. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **f** with the selected radical species in benzene.

f		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-75	289	-364	-150	76
	N2 (A)	-102		-391	-182	80
	N2 (B)	-35		-324	-80	44
	O1 (B)	-72		-361	-49	-22
$\cdot OC(CH_3)_3$	N1 (A)	-84	277	-361	-147	63
	N2 (A)	-111		-388	-179	68
	N2 (B)	-44		-321	-77	32
	O1 (B)	-81		-358	-46	-34
$\cdot OH$	N1 (A)	-144	241	-385	-171	28
	N2 (A)	-171		-412	-203	32
	N2 (B)	-104		-345	-100	-4
	O1 (B)	-141		-382	-70	-70
$\cdot OOH$	N1 (A)	-7	326	-333	-119	112
	N2 (A)	-34		-360	-151	117
	N2 (B)	33		-293	-48	81
	O1 (B)	-4		-329	-18	14
$\cdot OOCH_3$	N1 (A)	2	329	-327	-114	116
	N2 (A)	-25		-354	-146	120
	N2 (B)	42		-288	-43	84
	O1 (B)	5		-324	-13	18
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	281	-281	-67	67
	N2 (A)	-27		-308	-99	72
	N2 (B)	40		-241	4	36
	O1 (B)	3		-277	34	-30
DPPH	N1 (A)	21	182	-161	52	-32
	N2 (A)	-7		-189	20	-27
	N2 (B)	60		-122	123	-63
	O1 (B)	24		-158	153	-129
$O_2\cdot^-$	N1 (A)	89	812	-723	-23	112
	N2 (A)	62		-750	-55	117
	N2 (B)	129		-683	48	81
	O1 (B)	92		-720	78	14

Table S54. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **g** with the selected radical species in benzene.

g		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-75	288	-363	-149	74
	N2 (A)	-103		-391	-178	76
	N2 (B)	-36		-324	-78	43
	O1 (B)	-55		-343	-48	-7
$\cdot OC(CH_3)_3$	N1 (A)	-84	276	-360	-146	62
	N2 (A)	-112		-388	-175	64
	N2 (B)	-45		-321	-76	31
	O1 (B)	-64		-340	-45	-19
$\cdot OH$	N1 (A)	-144	240	-384	-170	26
	N2 (A)	-171		-411	-199	28
	N2 (B)	-104		-344	-99	-5
	O1 (B)	-124		-364	-69	-55
$\cdot OOH$	N1 (A)	-7	325	-332	-118	111
	N2 (A)	-35		-359	-147	112
	N2 (B)	32		-292	-47	80
	O1 (B)	13		-311	-17	30
$\cdot OOCH_3$	N1 (A)	2	328	-326	-112	114
	N2 (A)	-26		-354	-142	116
	N2 (B)	41		-287	-42	83
	O1 (B)	22		-306	-11	33
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	280	-280	-66	66
	N2 (A)	-27		-307	-95	68
	N2 (B)	40		-240	5	35
	O1 (B)	20		-260	35	-15
DPPH	N1 (A)	20	181	-160	54	-33
	N2 (A)	-7		-188	24	-31
	N2 (B)	60		-121	124	-64
	O1 (B)	41		-140	155	-114
$O_2^{\cdot -}$	N1 (A)	89	811	-722	-22	111
	N2 (A)	62		-749	-51	112
	N2 (B)	129		-682	49	80
	O1 (B)	109		-702	79	30

Table S55. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **h** with the selected radical species in benzene.

h		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-73	290	-363	-152	79
	N2 (A)	-97		-387	-176	80
	N2 (B)	-35		-325	-83	49
	O1 (B)	-51		-341	-94	43
$\cdot OC(CH_3)_3$	N1 (A)	-82	278	-360	-149	66
	N2 (A)	-106		-384	-173	68
	N2 (B)	-44		-322	-80	37
	O1 (B)	-60		-338	-91	31
$\cdot OH$	N1 (A)	-142	242	-384	-173	31
	N2 (A)	-166		-408	-197	32
	N2 (B)	-103		-345	-104	1
	O1 (B)	-120		-362	-115	-5
$\cdot OOH$	N1 (A)	-5	327	-332	-120	115
	N2 (A)	-29		-355	-145	116
	N2 (B)	33		-293	-52	85
	O1 (B)	17		-310	-63	80
$\cdot OOCH_3$	N1 (A)	4	330	-326	-115	119
	N2 (A)	-20		-350	-140	120
	N2 (B)	42		-288	-47	89
	O1 (B)	26		-304	-58	83
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	2	282	-280	-69	70
	N2 (A)	-22		-303	-93	72
	N2 (B)	41		-241	0	41
	O1 (B)	24		-258	-11	35
DPPH	N1 (A)	22	183	-161	51	-29
	N2 (A)	-1		-184	26	-27
	N2 (B)	61		-122	119	-58
	O1 (B)	44		-138	108	-64
$O_2^{\cdot -}$	N1 (A)	91	813	-722	-24	115
	N2 (A)	67		-746	-49	116
	N2 (B)	130		-683	44	85
	O1 (B)	113		-700	33	80

Table S56. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **i** with the selected radical species in benzene.

i		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-70	299	-370	-157	87
	N2 (A)	-97		-396	-186	89
	N2 (B)	-29		-328	-79	50
	O1 (B)	-71		-370	-58	-13
$\cdot OC(CH_3)_3$	N1 (A)	-80	287	-367	-154	75
	N2 (A)	-106		-393	-183	77
	N2 (B)	-38		-325	-76	38
	O1 (B)	-80		-367	-55	-25
$\cdot OH$	N1 (A)	-139	251	-390	-178	39
	N2 (A)	-166		-417	-207	41
	N2 (B)	-98		-349	-100	2
	O1 (B)	-140		-391	-79	-61
$\cdot OOH$	N1 (A)	-3	336	-338	-126	123
	N2 (A)	-29		-365	-154	125
	N2 (B)	39		-297	-47	86
	O1 (B)	-3		-339	-27	23
$\cdot OOCH_3$	N1 (A)	6	339	-333	-121	127
	N2 (A)	-20		-359	-149	129
	N2 (B)	48		-291	-42	90
	O1 (B)	6		-334	-21	27
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	5	291	-286	-74	79
	N2 (A)	-22		-313	-103	81
	N2 (B)	46		-245	4	42
	O1 (B)	4		-287	25	-21
DPPH	N1 (A)	25	192	-167	45	-20
	N2 (A)	-1		-193	17	-18
	N2 (B)	67		-125	124	-57
	O1 (B)	24		-168	145	-120
$O_2\cdot^-$	N1 (A)	94	822	-728	-30	123
	N2 (A)	67		-755	-58	125
	N2 (B)	135		-687	49	86
	O1 (B)	93		-729	70	23

Table S57. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **j** with the selected radical species in benzene.

j		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-74	299	-373	-161	87
	N2 (A)	-100		-399	-190	89
	N2 (B)	-33		-332	-89	56
	O1 (B)	-71		-370	-65	-6
$\cdot OC(CH_3)_3$	N1 (A)	-83	287	-370	-158	75
	N2 (A)	-109		-397	-187	77
	N2 (B)	-42		-329	-86	44
	O1 (B)	-80		-367	-62	-18
$\cdot OH$	N1 (A)	-143	251	-394	-182	39
	N2 (A)	-169		-420	-211	41
	N2 (B)	-102		-353	-110	8
	O1 (B)	-140		-391	-86	-54
$\cdot OOH$	N1 (A)	-6	336	-342	-129	124
	N2 (A)	-32		-368	-158	126
	N2 (B)	35		-301	-58	92
	O1 (B)	-3		-339	-34	31
$\cdot OOCH_3$	N1 (A)	3	339	-336	-124	127
	N2 (A)	-23		-363	-153	130
	N2 (B)	44		-296	-52	96
	O1 (B)	6		-333	-28	34
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	1	291	-290	-78	79
	N2 (A)	-25		-316	-106	81
	N2 (B)	42		-249	-6	48
	O1 (B)	4		-287	18	-14
DPPH	N1 (A)	22	192	-170	42	-20
	N2 (A)	-5		-197	13	-18
	N2 (B)	62		-130	114	-51
	O1 (B)	25		-167	138	-113
$O_2^{\cdot -}$	N1 (A)	90	822	-732	-33	124
	N2 (A)	64		-758	-62	126
	N2 (B)	131		-691	39	92
	O1 (B)	93		-729	63	31

Table S58. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **k** with the selected radical species in benzene.

k		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-75	284	-359	-145	70
	N2 (A)	-102		-386	-175	73
	N2 (B)	-36		-320	-74	38
	O1 (B)	-77		-362	-50	-27
$\cdot OC(CH_3)_3$	N1 (A)	-84	272	-356	-142	58
	N2 (A)	-111		-383	-172	60
	N2 (B)	-45		-317	-71	26
	O1 (B)	-86		-359	-47	-39
$\cdot OH$	N1 (A)	-144	236	-380	-166	22
	N2 (A)	-171		-407	-196	25
	N2 (B)	-105		-341	-95	-10
	O1 (B)	-146		-382	-71	-75
$\cdot OOH$	N1 (A)	-7	321	-328	-114	106
	N2 (A)	-34		-355	-143	109
	N2 (B)	32		-289	-43	74
	O1 (B)	-9		-330	-19	9
$\cdot OOCH_3$	N1 (A)	2	324	-323	-108	110
	N2 (A)	-25		-350	-138	113
	N2 (B)	41		-284	-37	78
	O1 (B)	-1		-325	-13	13
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	276	-276	-62	62
	N2 (A)	-27		-303	-92	65
	N2 (B)	39		-237	9	30
	O1 (B)	-2		-278	33	-35
DPPH	N1 (A)	20	177	-157	58	-37
	N2 (A)	-7		-184	28	-34
	N2 (B)	59		-118	129	-69
	O1 (B)	18		-159	153	-134
$O_2^{\cdot -}$	N1 (A)	89	807	-718	-17	106
	N2 (A)	62		-745	-47	109
	N2 (B)	128		-679	54	74
	O1 (B)	87		-720	77	9

Table S59. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **l** with the selected radical species in benzene.

l		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	282	-357	-143	67
	N2 (A)	-104		-386	-172	68
	N2 (B)	-37		-318	-74	37
	O1 (B)	-72		-353	-41	-31
$\cdot OC(CH_3)_3$	N1 (A)	-85	269	-355	-140	55
	N2 (A)	-113		-383	-169	56
	N2 (B)	-46		-315	-71	25
	O1 (B)	-81		-350	-38	-43
$\cdot OH$	N1 (A)	-145	233	-378	-164	19
	N2 (A)	-173		-407	-193	20
	N2 (B)	-106		-339	-95	-11
	O1 (B)	-141		-374	-62	-79
$\cdot OOH$	N1 (A)	-8	318	-326	-112	104
	N2 (A)	-36		-354	-141	104
	N2 (B)	31		-287	-42	73
	O1 (B)	-4		-322	-10	6
$\cdot OOCH_3$	N1 (A)	1	322	-321	-106	107
	N2 (A)	-27		-349	-135	108
	N2 (B)	40		-282	-37	77
	O1 (B)	5		-317	-4	9
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	273	-274	-60	59
	N2 (A)	-29		-302	-89	60
	N2 (B)	38		-235	10	29
	O1 (B)	3		-270	42	-39
DPPH	N1 (A)	20	174	-155	60	-40
	N2 (A)	-9		-183	31	-39
	N2 (B)	59		-116	129	-70
	O1 (B)	24		-151	162	-138
$O_2^{\cdot -}$	N1 (A)	88	804	-716	-15	104
	N2 (A)	60		-745	-44	104
	N2 (B)	127		-677	54	73
	O1 (B)	92		-712	86	6

Table S60. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **m** with the selected radical species in benzene.

m		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-74	275	-349	-143	69
	N2 (A)	-101		-377	-172	71
	N2 (B)	-35		-310	-62	27
	O1 (B)	-56		-331	-83	27
	O1 (C)	-112		-387	-152	41
	O2 (C)	-105		-380	-143	38
$\cdot OC(CH_3)_3$	N1 (A)	-84	263	-346	-140	57
	N2 (A)	-111		-374	-169	59
	N2 (B)	-44		-307	-59	15
	O1 (B)	-65		-328	-80	15
	O1 (C)	-121		-384	-150	29
	O2 (C)	-114		-377	-140	25
$\cdot OH$	N1 (A)	-143	227	-370	-164	21
	N2 (A)	-170		-397	-193	23
	N2 (B)	-104		-331	-83	-21
	O1 (B)	-125		-352	-104	-21
	O1 (C)	-181		-408	-173	-7
	O2 (C)	-174		-401	-164	-10
$\cdot OOH$	N1 (A)	-6	312	-318	-112	105
	N2 (A)	-34		-345	-141	107
	N2 (B)	33		-279	-31	64
	O1 (B)	12		-300	-52	64
	O1 (C)	-44		-356	-121	77
	O2 (C)	-37		-349	-111	74
$\cdot OOCH_3$	N1 (A)	2	315	-313	-106	109
	N2 (A)	-25		-340	-136	111
	N2 (B)	42		-273	-26	67
	O1 (B)	21		-294	-46	67
	O1 (C)	-35		-350	-116	81
	O2 (C)	-28		-343	-106	78
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	1	267	-266	-60	61
	N2 (A)	-26		-293	-89	63
	N2 (B)	40		-227	21	19
	O1 (B)	19		-248	0	19
	O1 (C)	-37		-304	-69	33
	O2 (C)	-30		-297	-59	30
DPPH	N1 (A)	21	168	-147	60	-38
	N2 (A)	-6		-174	30	-36
	N2 (B)	61		-107	140	-80
	O1 (B)	40		-128	120	-80
	O1 (C)	-16		-184	50	-66
	O2 (C)	-10		-178	60	-70
$O_2^{\cdot -}$	N1 (A)	90	798	-708	-15	105
	N2 (A)	63		-735	-45	107
	N2 (B)	129		-669	65	64
	O1 (B)	108		-690	45	64
	O1 (C)	52		-746	-25	77
	O2 (C)	59		-739	-15	74

Table S61. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **n** with the selected radical species in benzene.

n		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	279	-355	-144	68
	N2 (A)	-104		-383	-174	70
	N2 (B)	-37		-316	-71	34
	O1 (B)	-74		-353	-90	16
	O2 (C)	-105		-384	-134	29
	O3 (C)	-109		-388	-133	24
$\cdot OC(CH_3)_3$	N1 (A)	-85	267	-352	-141	55
	N2 (A)	-113		-380	-171	58
	N2 (B)	-46		-313	-68	22
	O1 (B)	-83		-350	-87	4
	O2 (C)	-114		-381	-131	17
	O3 (C)	-118		-385	-130	12
$\cdot OH$	N1 (A)	-145	231	-376	-165	20
	N2 (A)	-173		-404	-195	22
	N2 (B)	-105		-336	-92	-14
	O1 (B)	-143		-374	-111	-32
	O2 (C)	-174		-405	-155	-19
	O3 (C)	-178		-409	-154	-24
$\cdot OOH$	N1 (A)	-8	316	-324	-113	104
	N2 (A)	-36		-351	-142	106
	N2 (B)	31		-284	-39	71
	O1 (B)	-6		-321	-58	53
	O2 (C)	-37		-353	-103	66
	O3 (C)	-41		-357	-102	61
$\cdot OOCH_3$	N1 (A)	1	319	-319	-107	108
	N2 (A)	-27		-346	-137	110
	N2 (B)	40		-279	-34	74
	O1 (B)	3		-316	-53	56
	O2 (C)	-28		-347	-97	69
	O3 (C)	-32		-352	-97	64
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	271	-272	-61	60
	N2 (A)	-29		-300	-90	62
	N2 (B)	39		-232	13	26
	O1 (B)	1		-270	-6	8
	O2 (C)	-30		-301	-51	21
	O3 (C)	-34		-305	-50	16
DPPH	N1 (A)	19	172	-153	59	-39
	N2 (A)	-8		-180	29	-37
	N2 (B)	59		-113	132	-73
	O1 (B)	22		-150	113	-91
	O2 (C)	-10		-181	68	-78
	O3 (C)	-14		-186	69	-83
$O_2^{\cdot -}$	N1 (A)	88	802	-714	-16	104
	N2 (A)	60		-742	-46	106
	N2 (B)	128		-674	57	71
	O1 (B)	90		-712	38	53
	O2 (C)	59		-743	-7	66
	O3 (C)	55		-747	-6	61

Table S62. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **o** with the selected radical species in benzene.

o		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	272	-347	-140	64
	N2 (A)	-103		-375	-166	63
	N2 (B)	-38		-310	-68	29
	O1 (B)	-75		-346	-80	6
	O2 (C)	-87		-358	-109	22
$\cdot OC(CH_3)_3$	N1 (A)	-85	259	-344	-137	52
	N2 (A)	-112		-372	-163	50
	N2 (B)	-48		-307	-65	17
	O1 (B)	-84		-343	-77	-6
	O2 (C)	-96		-355	-106	10
$\cdot OH$	N1 (A)	-145	224	-368	-160	16
	N2 (A)	-172		-396	-187	15
	N2 (B)	-107		-331	-89	-19
	O1 (B)	-143		-367	-101	-42
	O2 (C)	-156		-379	-130	-26
$\cdot OOH$	N1 (A)	-8	308	-316	-108	101
	N2 (A)	-35		-343	-134	99
	N2 (B)	29		-279	-36	66
	O1 (B)	-7		-315	-49	42
	O2 (C)	-19		-327	-78	59
$\cdot OOCH_3$	N1 (A)	1	312	-310	-103	104
	N2 (A)	-26		-338	-129	103
	N2 (B)	38		-273	-31	69
	O1 (B)	2		-309	-44	46
	O2 (C)	-10		-322	-72	63
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	264	-264	-56	56
	N2 (A)	-28		-292	-82	54
	N2 (B)	37		-227	16	21
	O1 (B)	1		-263	3	-2
	O2 (C)	-12		-275	-26	14
DPPH	N1 (A)	20	165	-145	63	-43
	N2 (A)	-8		-172	37	-45
	N2 (B)	57		-107	135	-78
	O1 (B)	21		-144	122	-101
	O2 (C)	9		-156	93	-85
$O_2^{\cdot -}$	N1 (A)	89	795	-706	-12	101
	N2 (A)	61		-734	-38	99
	N2 (B)	126		-669	60	66
	O1 (B)	90		-705	47	42
	O2 (C)	77		-717	18	59

Table S63. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **p** with the selected radical species in benzene.

p		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	304	-380	-148	73
	N2 (A)	-103		-408	-172	69
	N2 (B)	-37		-341	-78	41
	O1 (B)	-47		-351	-44	-3
	O3 (C)	-82		-386	-82	0
$\cdot OC(CH_3)_3$	N1 (A)	-85	292	-377	-145	61
	N2 (A)	-113		-405	-169	57
	N2 (B)	-46		-338	-75	29
	O1 (B)	-56		-348	-41	-15
	O3 (C)	-91		-383	-79	-12
$\cdot OH$	N1 (A)	-144	256	-401	-169	25
	N2 (A)	-172		-429	-193	21
	N2 (B)	-106		-362	-99	-7
	O1 (B)	-116		-372	-65	-51
	O3 (C)	-151		-407	-103	-48
$\cdot OOH$	N1 (A)	-8	341	-348	-117	109
	N2 (A)	-36		-376	-141	105
	N2 (B)	31		-310	-46	77
	O1 (B)	21		-320	-13	34
	O3 (C)	-14		-355	-50	37
$\cdot OOCH_3$	N1 (A)	1	344	-343	-112	113
	N2 (A)	-27		-371	-136	109
	N2 (B)	40		-304	-41	81
	O1 (B)	30		-314	-7	37
	O3 (C)	-5		-349	-45	40
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	296	-297	-65	65
	N2 (A)	-28		-324	-89	61
	N2 (B)	38		-258	6	33
	O1 (B)	28		-268	39	-11
	O3 (C)	-7		-303	2	-8
DPPH	N1 (A)	20	197	-177	54	-34
	N2 (A)	-8		-205	30	-38
	N2 (B)	59		-138	125	-66
	O1 (B)	49		-148	159	-110
	O3 (C)	14		-183	121	-107
$O_2^{\cdot -}$	N1 (A)	89	827	-739	-21	109
	N2 (A)	61		-767	-45	105
	N2 (B)	127		-700	50	77
	O1 (B)	117		-710	83	34
	O3 (C)	82		-745	46	37

Table S64. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **q** with the selected radical species in benzene.

q		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	290	-366	-148	71
	N2 (A)	-105		-394	-177	73
	N2 (B)	-37		-327	-76	39
	O1 (B)	-74		-363	-98	24
	O3 (C)	-98		-388	-78	-20
$\cdot OC(CH_3)_3$	N1 (A)	-86	277	-363	-145	59
	N2 (A)	-114		-391	-174	60
	N2 (B)	-46		-324	-73	27
	O1 (B)	-83		-360	-95	12
	O3 (C)	-107		-385	-75	-33
$\cdot OH$	N1 (A)	-145	242	-387	-169	23
	N2 (A)	-173		-415	-198	25
	N2 (B)	-106		-347	-97	-9
	O1 (B)	-143		-384	-119	-24
	O3 (C)	-167		-409	-98	-68
$\cdot OOH$	N1 (A)	-9	326	-335	-117	108
	N2 (A)	-37		-363	-146	109
	N2 (B)	31		-295	-45	76
	O1 (B)	-6		-332	-67	61
	O3 (C)	-30		-356	-46	16
$\cdot OOCH_3$	N1 (A)	0	330	-329	-111	111
	N2 (A)	-28		-357	-140	113
	N2 (B)	40		-290	-39	79
	O1 (B)	3		-327	-61	64
	O3 (C)	-21		-351	-41	20
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	282	-283	-65	63
	N2 (A)	-29		-311	-94	65
	N2 (B)	38		-243	7	31
	O1 (B)	2		-280	-15	16
	O3 (C)	-23		-304	6	-28
DPPH	N1 (A)	19	183	-163	55	-36
	N2 (A)	-9		-192	26	-35
	N2 (B)	59		-124	126	-68
	O1 (B)	22		-161	105	-83
	O3 (C)	-2		-185	125	-128
$O_2^{\cdot -}$	N1 (A)	88	813	-725	-20	108
	N2 (A)	60		-753	-50	109
	N2 (B)	127		-685	51	76
	O1 (B)	90		-722	30	61
	O3 (C)	66		-747	50	16

Table S65. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **r** with the selected radical species in benzene.

r		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-75	285	-360	-146	72
	N2 (A)	-102		-387	-174	72
	N2 (B)	-39		-324	-79	40
	O1 (B)	-47		-332	-46	-2
	O2 (C)	-86		-371	-110	24
$\cdot OC(CH_3)_3$	N1 (A)	-84	273	-357	-143	59
	N2 (A)	-112		-384	-171	60
	N2 (B)	-48		-321	-76	28
	O1 (B)	-57		-329	-43	-14
	O2 (C)	-95		-368	-107	12
$\cdot OH$	N1 (A)	-144	237	-380	-167	24
	N2 (A)	-171		-408	-195	24
	N2 (B)	-108		-345	-100	-8
	O1 (B)	-116		-353	-67	-50
	O2 (C)	-155		-392	-131	-24
$\cdot OOH$	N1 (A)	-7	321	-328	-115	108
	N2 (A)	-35		-356	-143	108
	N2 (B)	29		-293	-48	77
	O1 (B)	21		-301	-14	35
	O2 (C)	-18		-340	-79	61
$\cdot OOCH_3$	N1 (A)	2	325	-323	-110	112
	N2 (A)	-26		-351	-138	112
	N2 (B)	38		-287	-42	80
	O1 (B)	29		-295	-9	38
	O2 (C)	-9		-334	-74	64
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	0	277	-276	-63	64
	N2 (A)	-27		-304	-91	64
	N2 (B)	36		-241	4	32
	O1 (B)	28		-249	38	-10
	O2 (C)	-11		-288	-27	16
DPPH	N1 (A)	21	178	-157	56	-36
	N2 (A)	-7		-185	28	-35
	N2 (B)	56		-121	123	-67
	O1 (B)	48		-129	157	-109
	O2 (C)	9		-168	92	-83
$O_2^{\cdot -}$	N1 (A)	89	808	-718	-19	108
	N2 (A)	62		-746	-47	108
	N2 (B)	125		-683	48	77
	O1 (B)	117		-691	82	35
	O2 (C)	78		-730	17	61

Table S66. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **s** with the selected radical species in benzene.

s		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-76	281	-357	-147	71
	N2 (A)	-104		-385	-177	72
	N2 (B)	-37		-318	-78	41
	O1 (B)	-73		-354	-42	-31
$\cdot OC(CH_3)_3$	N1 (A)	-85	269	-354	-144	59
	N2 (A)	-113		-382	-174	60
	N2 (B)	-46		-315	-75	28
	O1 (B)	-82		-351	-39	-43
$\cdot OH$	N1 (A)	-145	233	-378	-168	23
	N2 (A)	-173		-406	-198	24
	N2 (B)	-106		-339	-99	-7
	O1 (B)	-142		-375	-63	-79
$\cdot OOH$	N1 (A)	-8	317	-325	-116	108
	N2 (A)	-36		-354	-145	109
	N2 (B)	31		-287	-47	77
	O1 (B)	-5		-323	-11	6
$\cdot OOCH_3$	N1 (A)	1	321	-320	-110	111
	N2 (A)	-27		-348	-140	113
	N2 (B)	40		-281	-41	81
	O1 (B)	4		-317	-6	9
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	-1	273	-273	-64	63
	N2 (A)	-29		-302	-93	64
	N2 (B)	38		-235	5	33
	O1 (B)	2		-271	41	-39
DPPH	N1 (A)	20	174	-154	56	-36
	N2 (A)	-9		-182	26	-35
	N2 (B)	58		-115	125	-66
	O1 (B)	22		-151	160	-138
$O_2^{\cdot -}$	N1 (A)	88	804	-716	-20	108
	N2 (A)	60		-744	-49	109
	N2 (B)	127		-677	50	77
	O1 (B)	91		-713	85	6

Table S67. Calculated reaction enthalpies (kJ mol $^{-1}$) for the reactions of compound **t** with the selected radical species in benzene.

t		HAT	SET-PT		SPLET	
Radical		ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$\cdot OCH_3$	N1 (A)	-73	286	-360	-152	79
	N2 (A)	-100		-387	-180	79
	N2 (B)	-35		-321	-80	45
	O1 (B)	-75		-362	-98	23
	O1 (C)	-81		-367	-160	79
$\cdot OC(CH_3)_3$	N1 (A)	-83	274	-357	-149	67
	N2 (A)	-110		-384	-177	67
	N2 (B)	-44		-318	-77	33
	O1 (B)	-84		-359	-95	11
	O1 (C)	-90		-364	-157	67
$\cdot OH$	N1 (A)	-142	238	-381	-173	31
	N2 (A)	-169		-408	-200	31
	N2 (B)	-104		-342	-101	-3
	O1 (B)	-144		-382	-119	-25
	O1 (C)	-150		-388	-181	31
$\cdot OOH$	N1 (A)	-5	323	-328	-121	115
	N2 (A)	-33		-355	-148	116
	N2 (B)	33		-290	-48	82
	O1 (B)	-7		-330	-67	60
	O1 (C)	-13		-336	-129	116
$\cdot OOCH_3$	N1 (A)	3	326	-323	-115	119
	N2 (A)	-24		-350	-143	119
	N2 (B)	42		-284	-43	85
	O1 (B)	2		-325	-62	63
	O1 (C)	-4		-330	-123	119
$\cdot OO\text{-}CH{=}CH_2$	N1 (A)	2	278	-276	-69	71
	N2 (A)	-25		-304	-96	71
	N2 (B)	40		-238	4	37
	O1 (B)	0		-278	-15	15
	O1 (C)	-6		-284	-77	71
DPPH	N1 (A)	22	179	-157	51	-28
	N2 (A)	-5		-184	23	-28
	N2 (B)	61		-118	123	-62
	O1 (B)	20		-159	104	-84
	O1 (C)	15		-165	42	-28
$O_2^{\cdot -}$	N1 (A)	91	809	-719	-25	115
	N2 (A)	64		-746	-52	116
	N2 (B)	129		-680	48	82
	O1 (B)	89		-720	29	60
	O1 (C)	83		-726	-33	116

Table S68. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **a.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	20	0.111	-90	-97
O	27	0.101	/	/
N	32	0.074	/	/
C	10	0.073	-57	-58
C	11	0.067	-66	-65
C	26	0.065	-54	-35
O	30	0.062	/	/
N	28	0.060	/	/

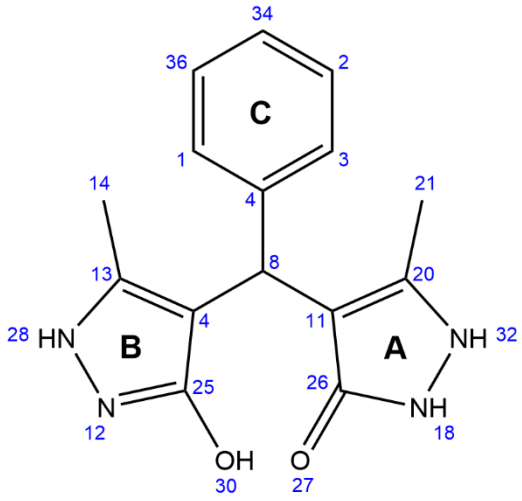


Table S69. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **b.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	19	0.102	-89	-85
O	26	0.081	/	/
N	31	0.068	/	/
C	10	0.057	-66	-67
O	29	0.054	/	/

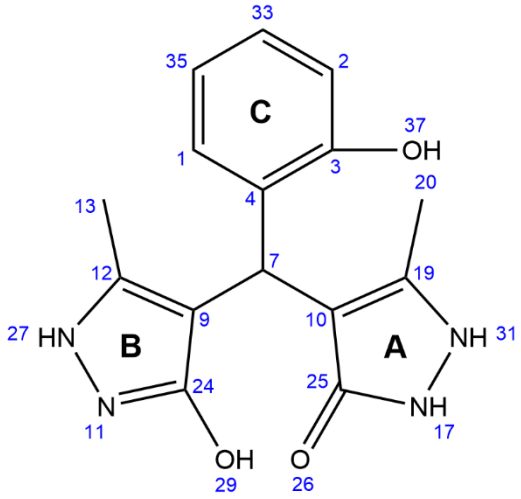


Table S70. Calculated Fukui function values for the radical attack ($f_{nbo}{}^0$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **c.**

Atom	Number	$f_{nbo}{}^0$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	20	0.111	-89	-97
O	27	0.101	/	/
N	32	0.074	/	/
C	10	0.073	-56	-59
C	11	0.067	-65	-65
O	30	0.062	/	/
C	26	0.061	-58	-38
N	28	0.059	/	/

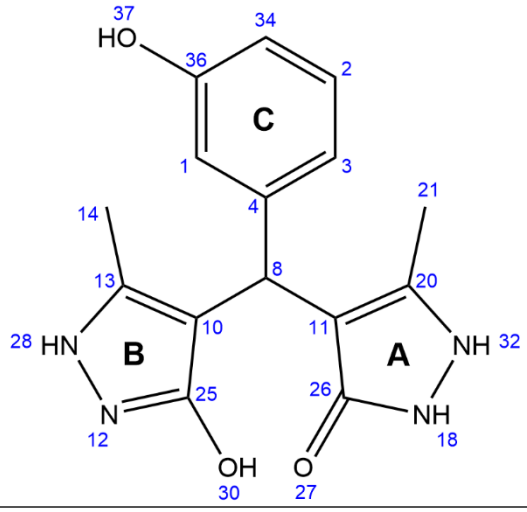


Table S71. Calculated Fukui function values for the radical attack ($f_{nbo}{}^0$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **d.**

Atom	Number	$f_{nbo}{}^0$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	20	0.089	-90	-97
N	32	0.089	/	/
O	27	0.086	/	/
C	11	0.076	-66	-67
C	10	0.076	-58	-58

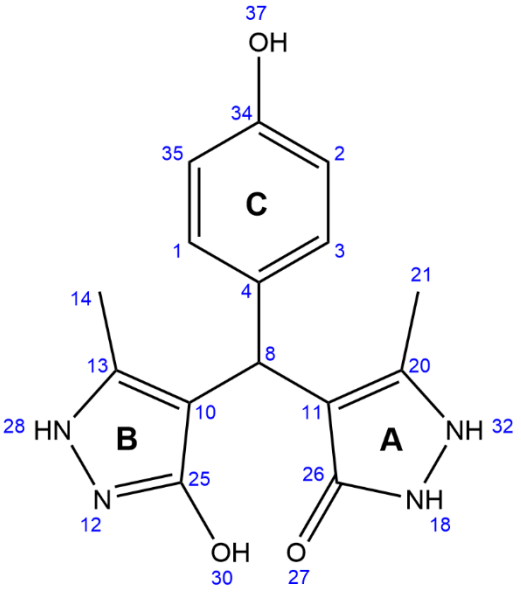


Table S72. Calculated Fukui function values for the radical attack ($f_{nbo}{}^0$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **e.**

Atom	Number	$f_{nbo}{}^0$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
O	26	0.076	/	/
C	9	0.071	-57	-56
C	3	0.068	-77	-75
C	35	0.066	-62	-55
C	19	0.062	-89	-96
O	29	0.061	/	/
N	27	0.059	/	/
C	1	0.058	-72	-71
N	31	0.055	/	/
C	10	0.055	-65	-65

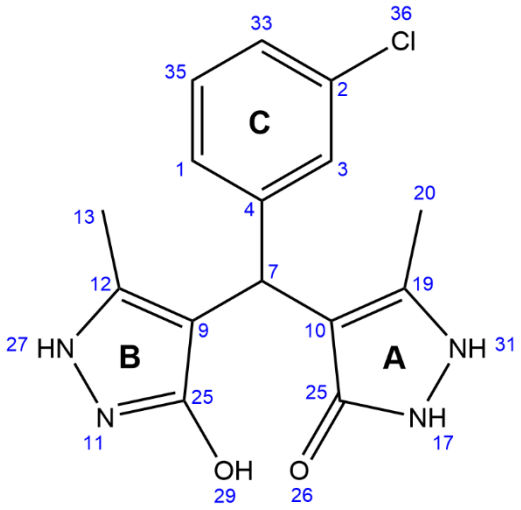


Table S73. Calculated Fukui function values for the radical attack ($f_{nbo}{}^0$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **f.**

Atom	Number	$f_{nbo}{}^0$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	2	0.085	-68	-66
C	1	0.077	-69	-66
O	27	0.075	/	/
C	10	0.073	-56	-99
O	30	0.060	/	/
C	20	0.058	-90	-96
N	28	0.058	/	/

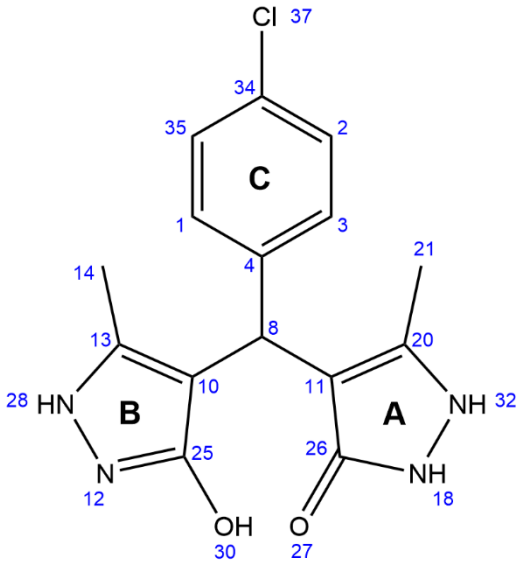


Table S74. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **g.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
O	27	0.075	/	/
C	2	0.075	-66	-61
C	10	0.073	-57	-99
C	1	0.068	-58	-66
C	35	0.064	-64	-60
O	30	0.061	/	/
C	20	0.060	-90	-97
N	28	0.058	/	/
C	3	0.058	-70	-67
C	11	0.055	-65	-66

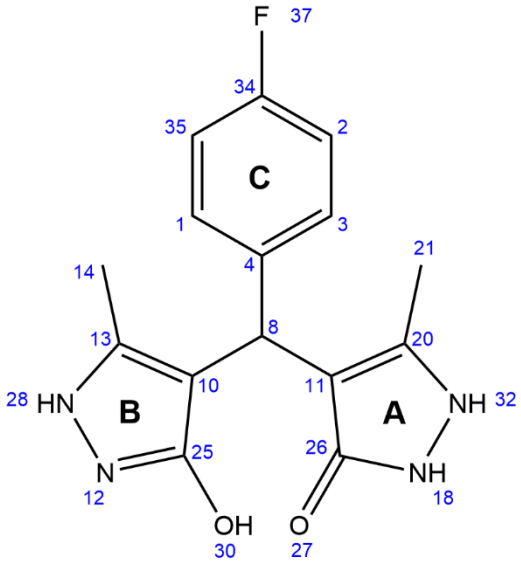


Table S75. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **h.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	9	0.069	-40	-42
O	29	0.065	/	/
N	27	0.061	/	/
O	26	0.054	/	/

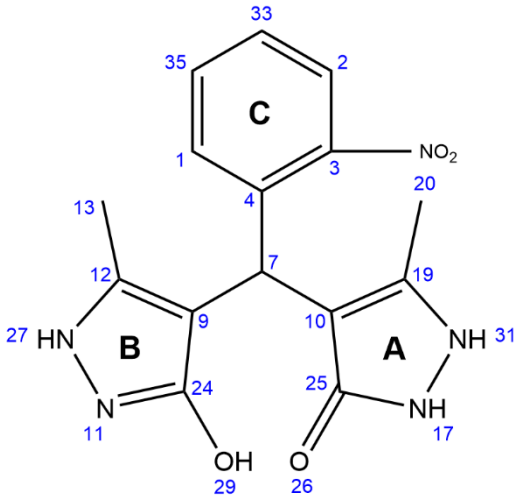


Table S76. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **i.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	10	0.071	-102	-57
O	30	0.061	/	/
N	28	0.059	/	/

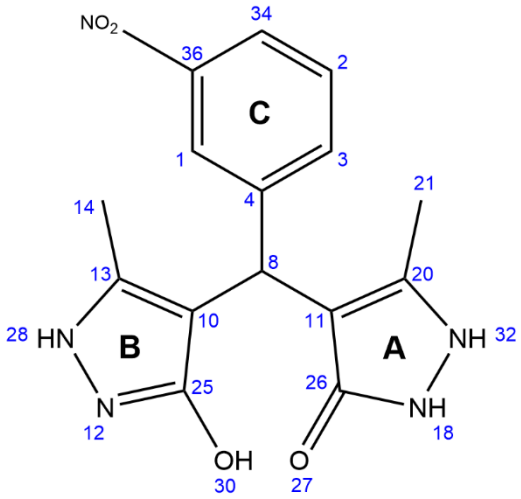


Table S77. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **j.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	10	0.071	-100	-57
O	30	0.058	/	/
N	28	0.056	/	/
O	27	0.056	/	/

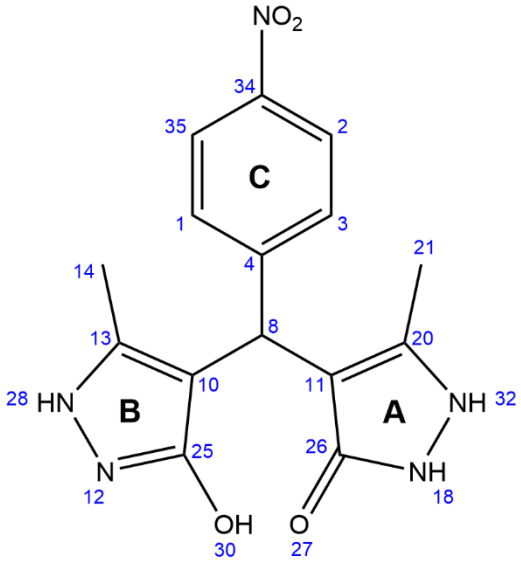


Table S78. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **k.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	19	0.122	-88	-98
O	26	0.110	/	/
N	31	0.082	/	/
C	10	0.076	-57	-57
C	25	0.070	-57	-39
C	9	0.067	-52	-53

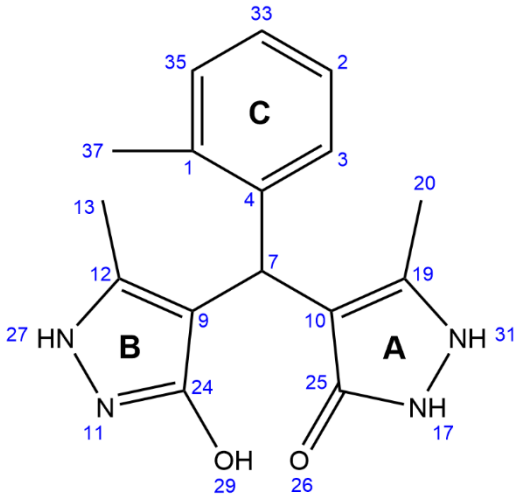


Table S79. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **l.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	20	0.109	-90	-98
O	27	0.102	/	/
C	10	0.075	-57	-58
N	32	0.074	/	/
C	11	0.067	-66	-66
C	26	0.061	-54	-34
O	30	0.061	/	/
N	28	0.059	/	/

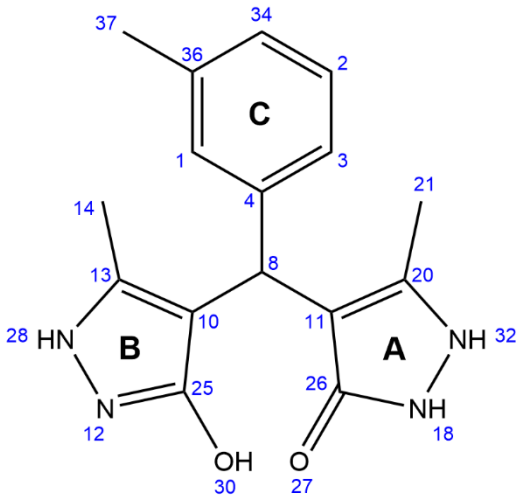


Table S80. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **m.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	19	0.115	-87	-95
C	2	0.080	-70	-64
C	25	0.071	-56	-40
C	1	0.070	-84	-78
O	36	0.063	/	/
C	35	0.061	-84	-89
O	26	0.060	/	/

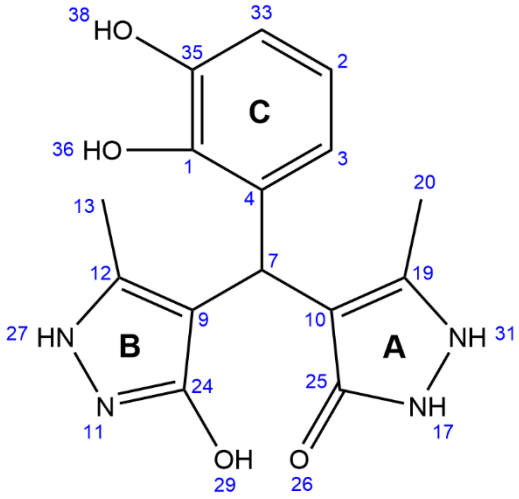


Table S81. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **n.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	22	0.105	-90	-98
C	3	0.075	-88	-92
C	6	0.071	-75	-75
C	5	0.070	-75	-73
C	28	0.065	-53	-37
O	32	0.062	/	/
C	2	0.060	-90	-80
O	29	0.058	/	/
O	30	0.057	/	/

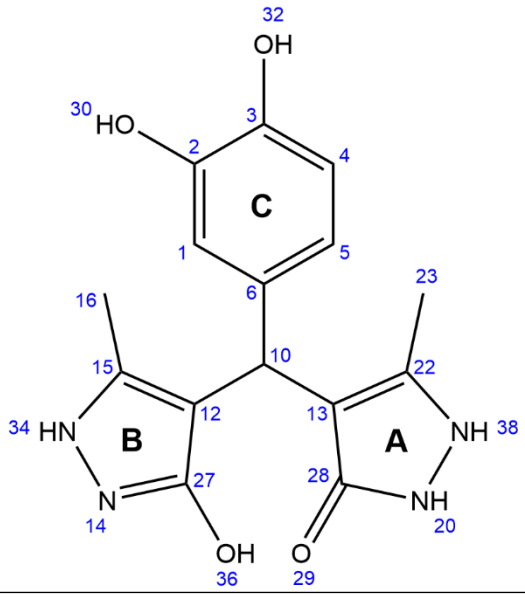


Table S82. Calculated Fukui function values for the radical attack ($f_{nbo}{}^0$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **o.**

Atom	Number	$f_{nbo}{}^0$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	18	0.112	-88	-86
C	34	0.079	-71	-63
C	1	0.071	-68	-68
C	3	0.070	-88	-80
C	2	0.066	-81	-82
O	36	0.063	/	/
O	38	0.061	/	/
C	24	0.061	-63	-42

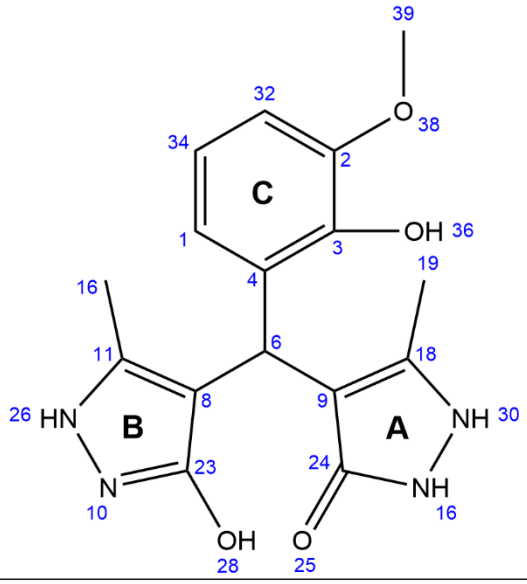


Table S83. Calculated Fukui function values for the radical attack ($f_{nbo}{}^0$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **p.**

Atom	Number	$f_{nbo}{}^0$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	20	0.108	-91	-97
C	4	0.075	-79	-74
C	34	0.074	-95	-85
C	26	0.067	-56	-30
O	36	0.066	/	/
C	3	0.063	-76	-72
O	27	0.058	/	/
C	35	0.056	-84	-79
O	38	0.055	/	/

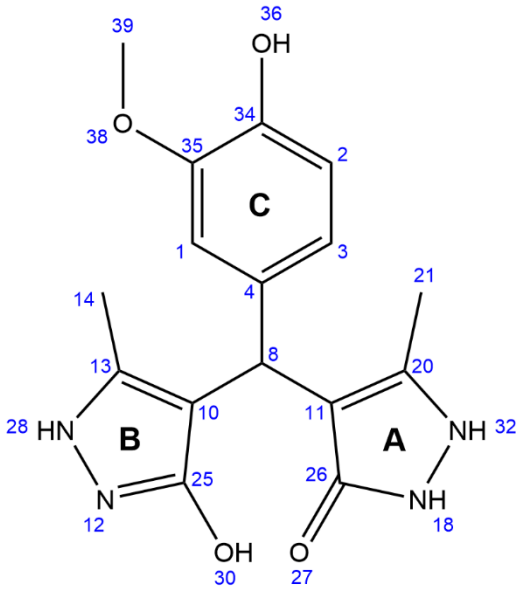


Table S84. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **q.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	19	0.112	-91	-98
C	33	0.089	-106	-103
O	36	0.072	/	/
C	25	0.071	-54	-38
C	3	0.061	-71	-71
O	26	0.061	/	/

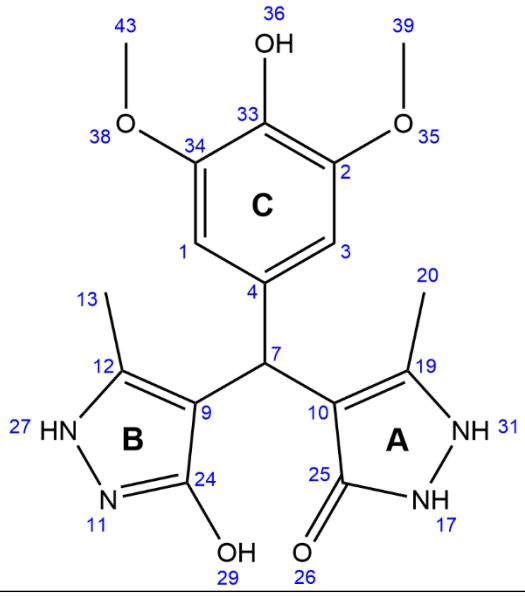


Table S85. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **r.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	17	0.119	-90	-97
O	24	0.104	/	/
N	29	0.076	/	/
C	7	0.072	-57	-55
C	8	0.068	-66	-67
C	23	0.068	-56	-30
O	27	0.059	/	/
N	25	0.058	/	/

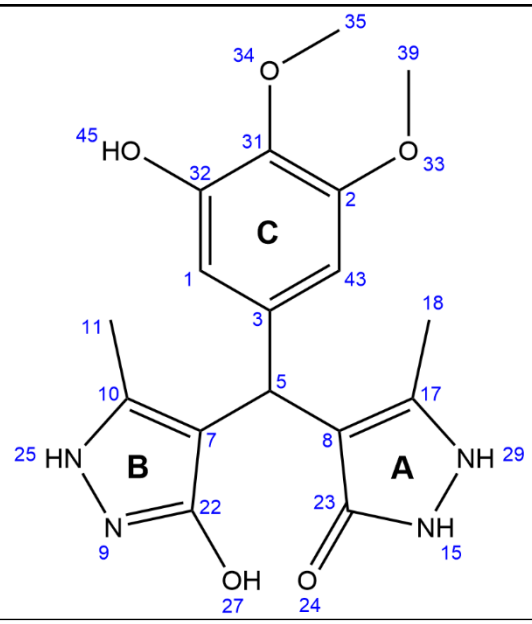


Table S86. Calculated Fukui function values for the radical attack ($f_{nbo}{}^{0}$) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **s.**

Atom	Number	$f_{nbo}{}^{0}$	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	19	0.115	-87	-98
O	26	0.103	/	/
N	31	0.101	/	/
C	10	0.066	-66	-69
C	25	0.062	-54	-36
N	17	0.057	/	/
C	9	0.056	-57	-59

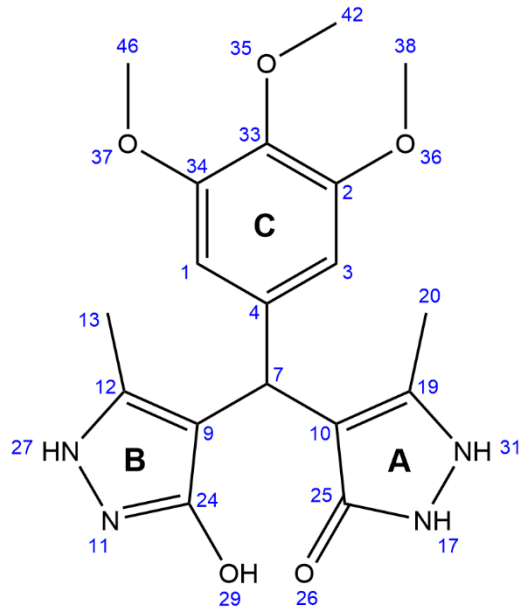


Table S87. Calculated Fukui function values for the radical attack (f_{nbo}^{0}) on the selected positions and ΔH_{RAF} values (kJ mol^{-1}) for compound **t.**

Atom	Number	f_{nbo}^{0}	ΔH_{RAF} (methanol)	ΔH_{RAF} (benzene)
C	32	0.106	-77	-72
C	1	0.075	-71	-66
O	28	0.068	/	/
C	4	0.066	-85	-77
C	8	0.062	-55	-56
N	26	0.060	/	/
O	25	0.058	/	/

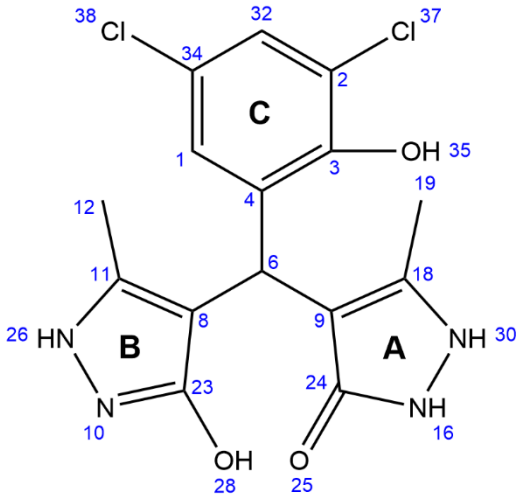


Table S88. Regresion equations parameters calculated by DPPH assay for compounds **a–t** and parent pyrazolone.

Analogue	**Regression equation**	**Corelation coefficient (r)**
a	y = 7.4716x + 11.814	0.9933
b	y = 5.1045x + 18.599	0.9769
c	y = 7.1268x + 19.769	0.9622
d	y = 8.8059x + 7.396	0.9943
e	y = 4.9523x + 27.897	0.9839
f	y = 5.7368x + 19.343	0.9862
g	y = 8.9619x + 6.8912	0.9821
h	y = 3.848x + 19.901	0.9866
i	y = 6.2356x + 22.023	0.9800
j	y = 3.4101x + 32.596	0.9909
k	y = 8.7339x + 13.068	0.9472
l	y = 7.8414x + 22.555	0.9786
m	y = 18.958x – 0.1678	0.9939
n	y = 17.47x – 1.2657	0.9981
o	y = 11.755x + 7.5286	0.9966
p	y = 7.5674x + 4.1716	0.9988
q	y = 7.7734x + 6.7145	0.9853

r	y = 6.5257x + 21.87	0.9760
s	y = 6.4569x + 9.9444	0.9846
t	y = 5.4435x + 14.961	0.9631
Pyrazolone	y = 2.5555x + 26.289	0.9811

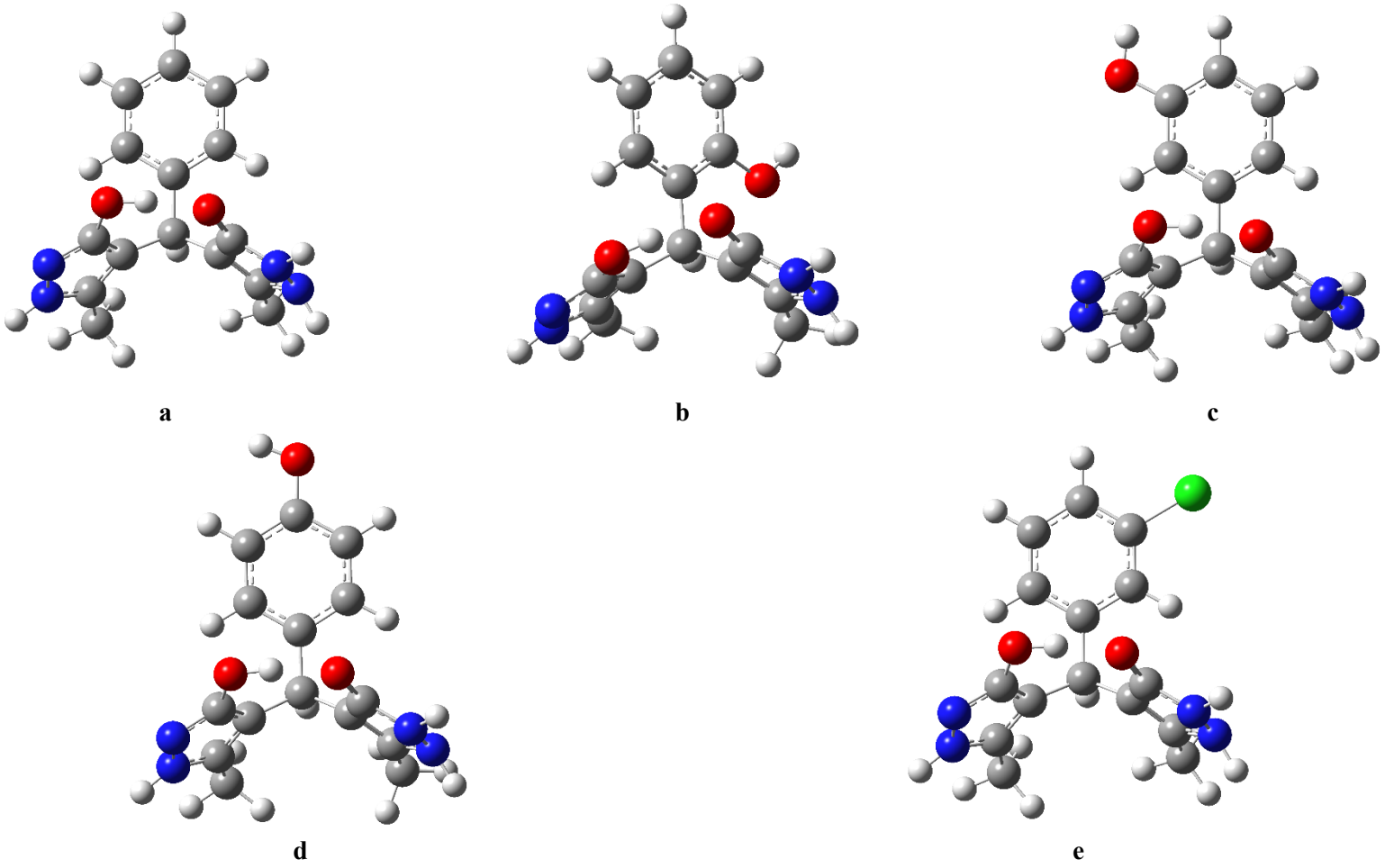


Figure S1. Optimized geometries of compounds **a–e** in methanol.

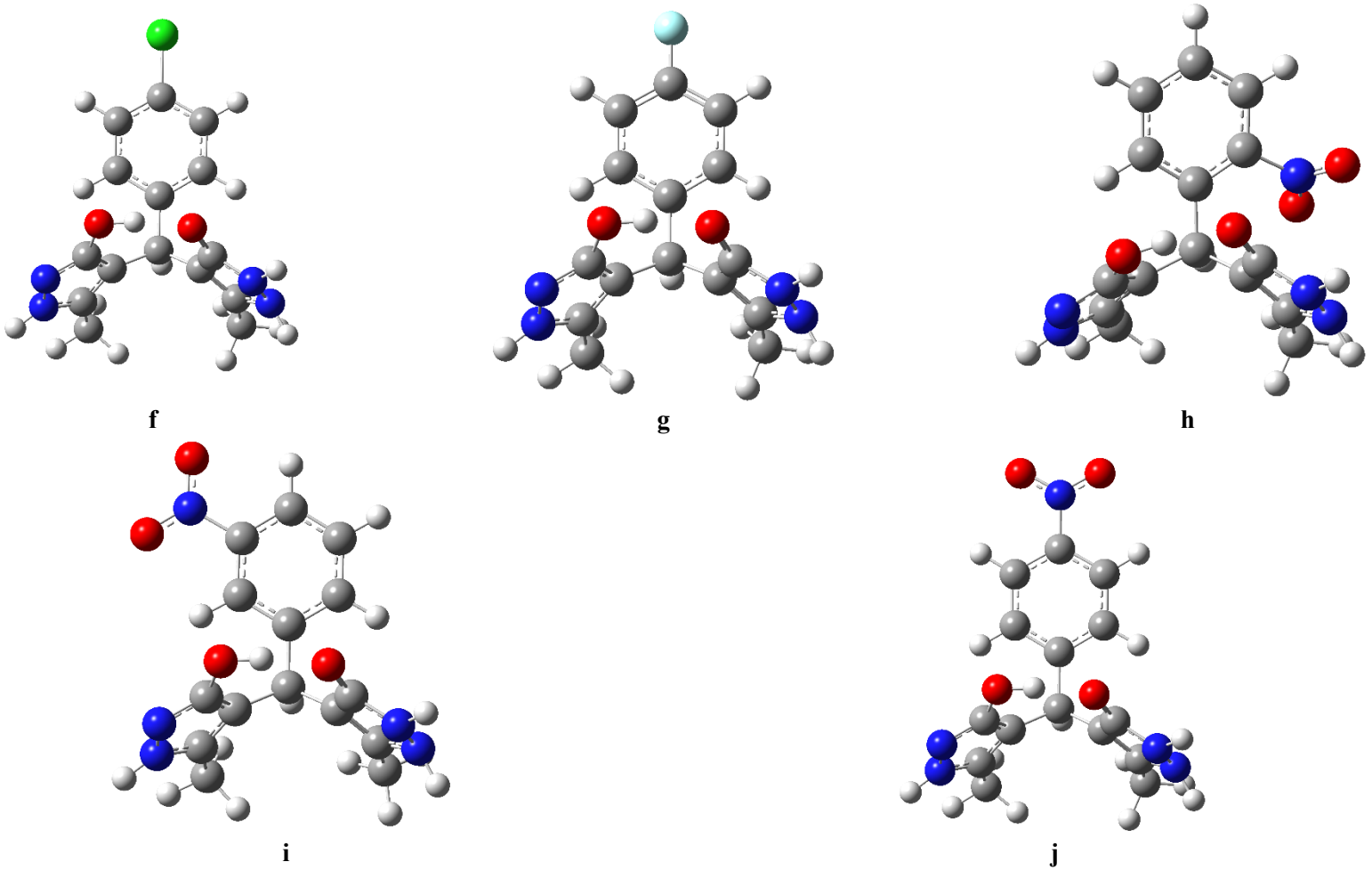


Figure S2. Optimized geometries of compounds **f–j** in methanol.

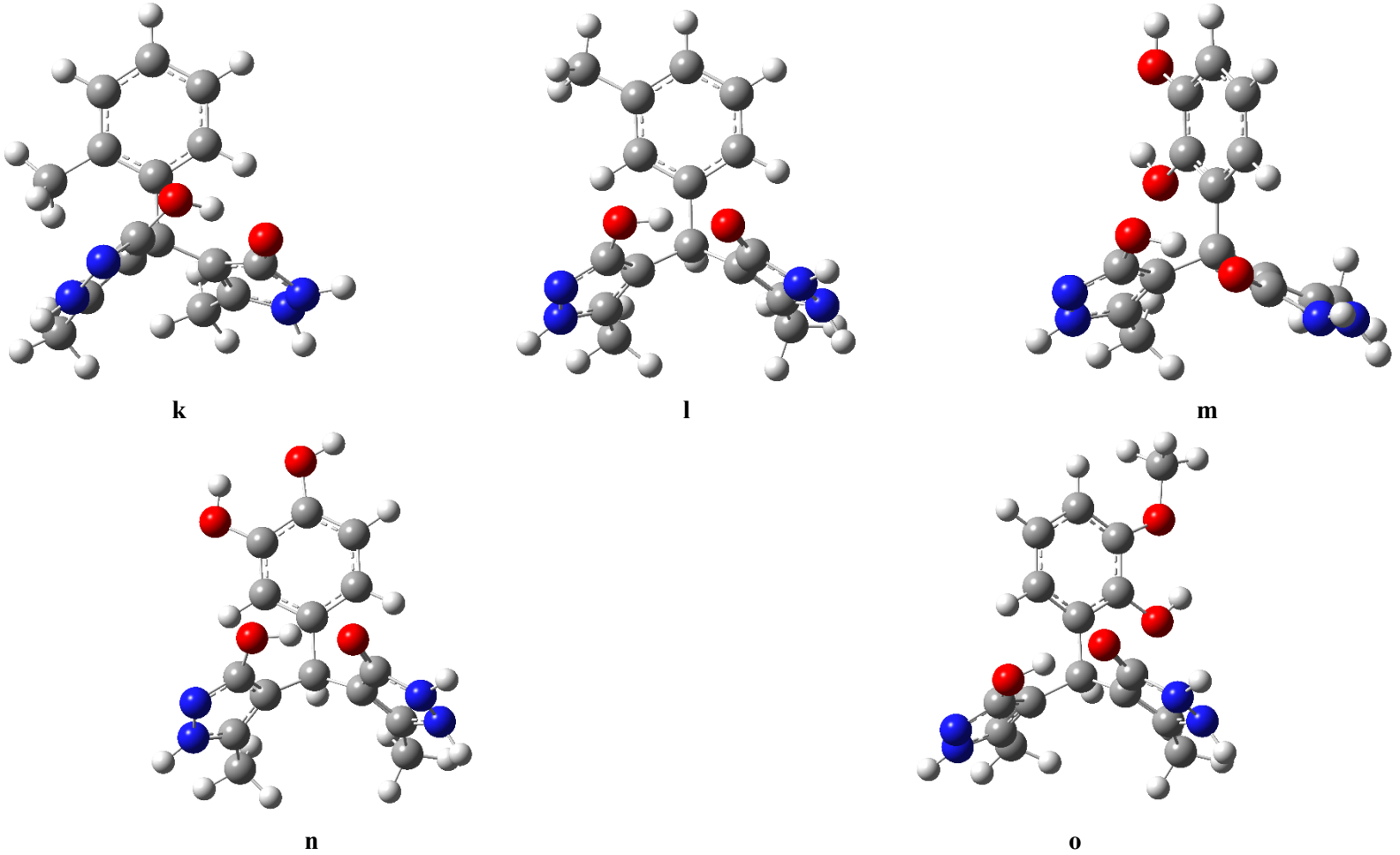


Figure S3. Optimized geometries of compounds **k–o** in methanol.

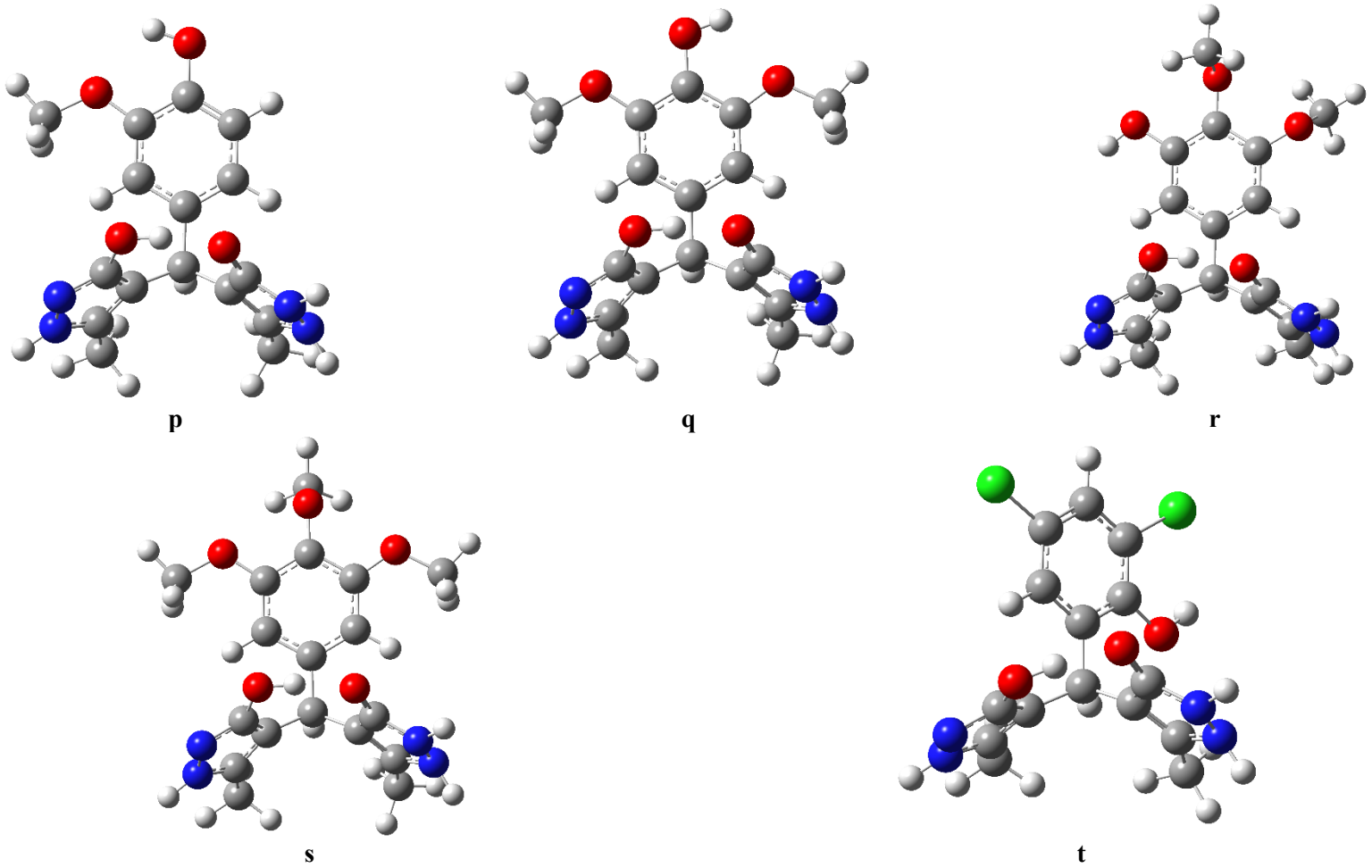


Figure S4. Optimized geometries of compounds **p–t** in methanol.

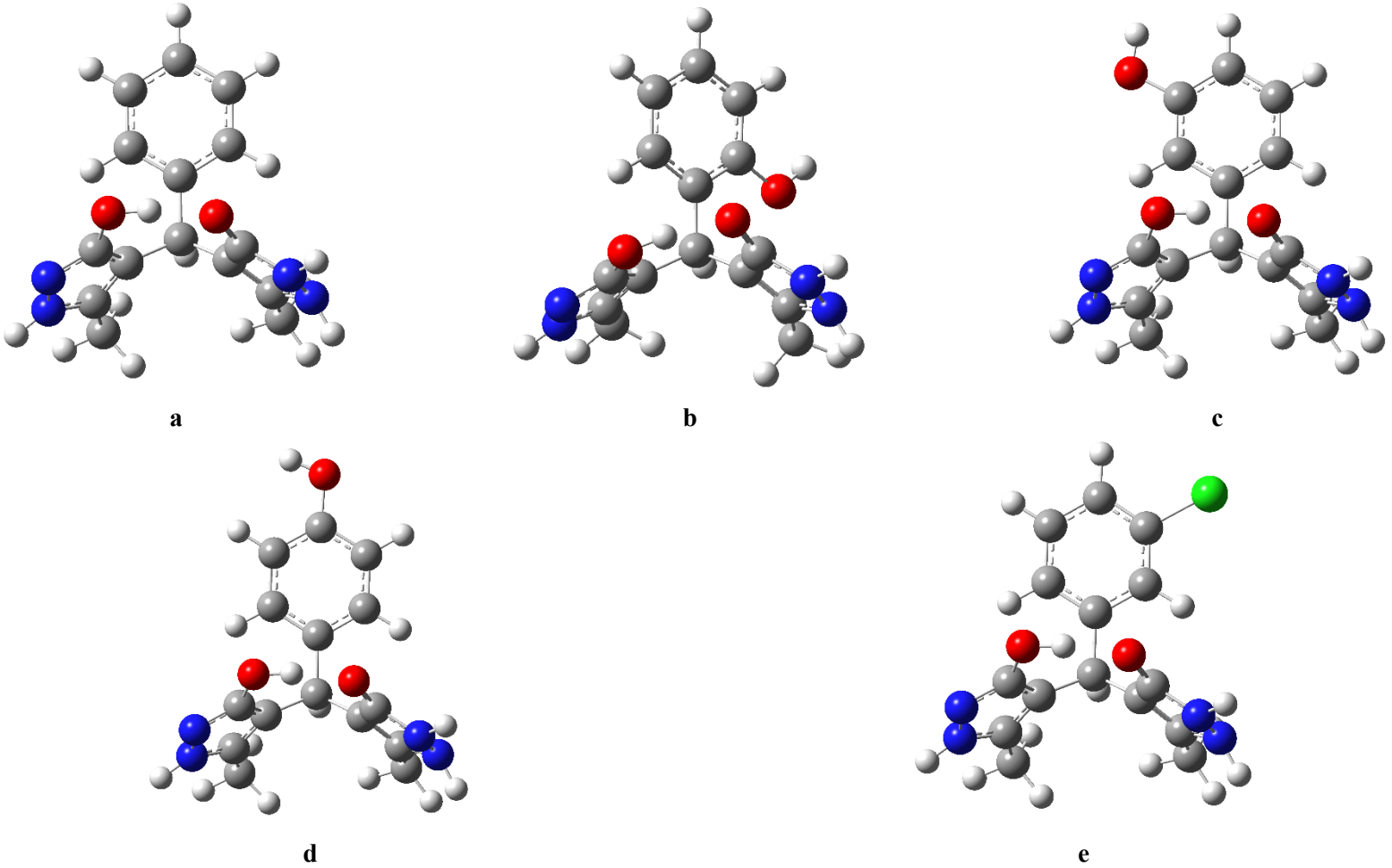


Figure S5. Optimized geometries of compounds **a–e** in water.

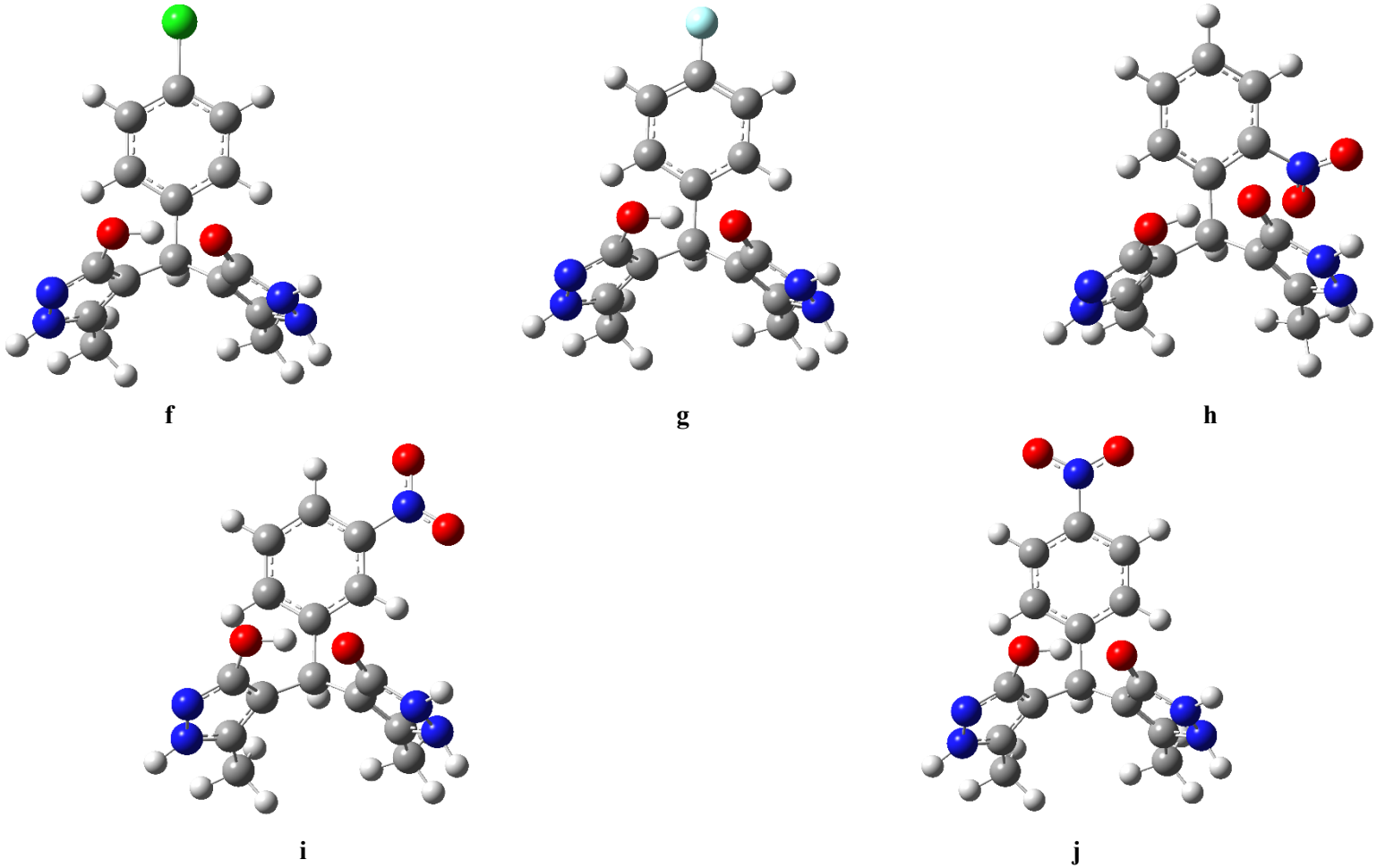


Figure S6. Optimized geometries of compounds **f–j** in water.

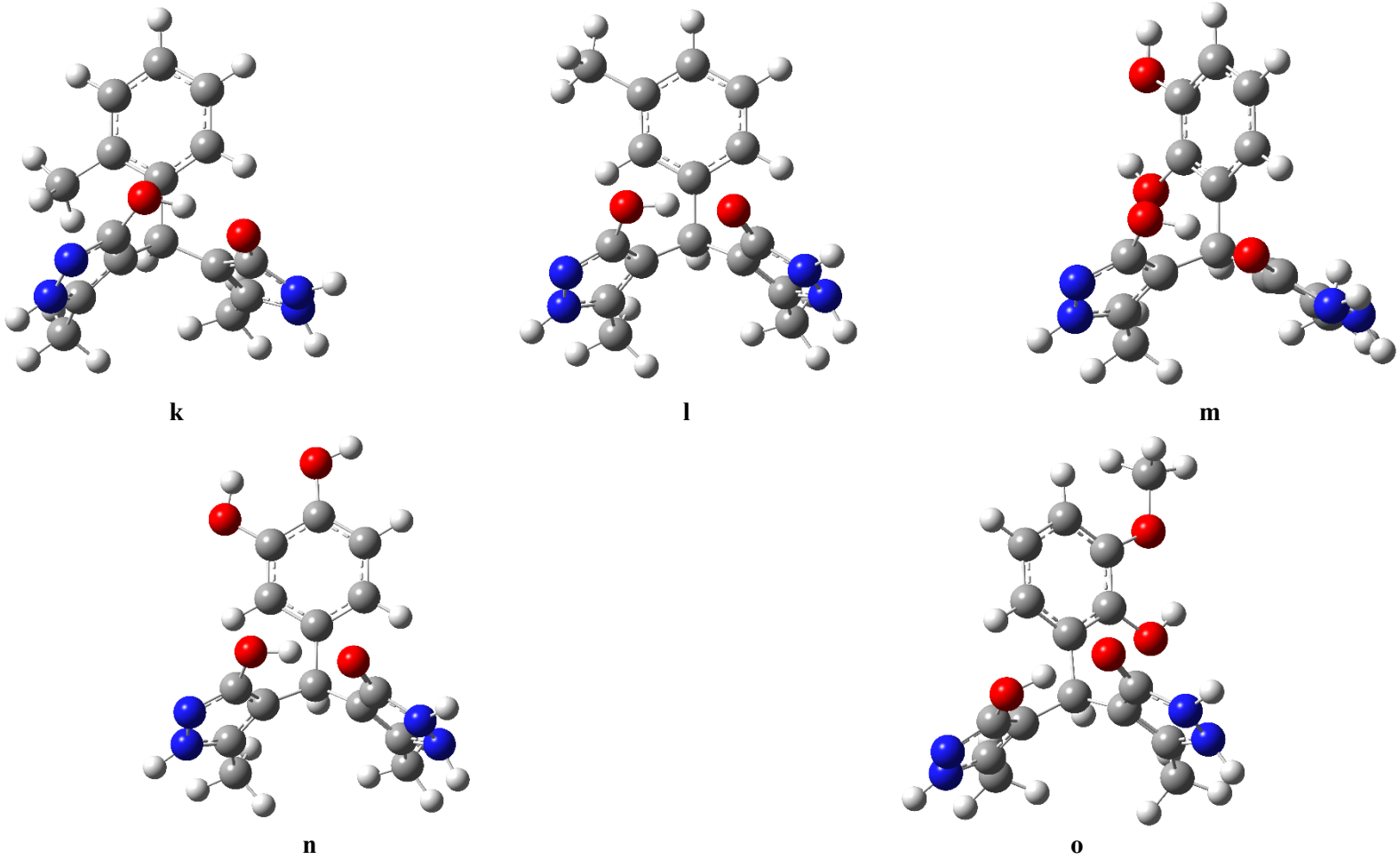


Figure S7. Optimized geometries of compounds **k–o** in water.

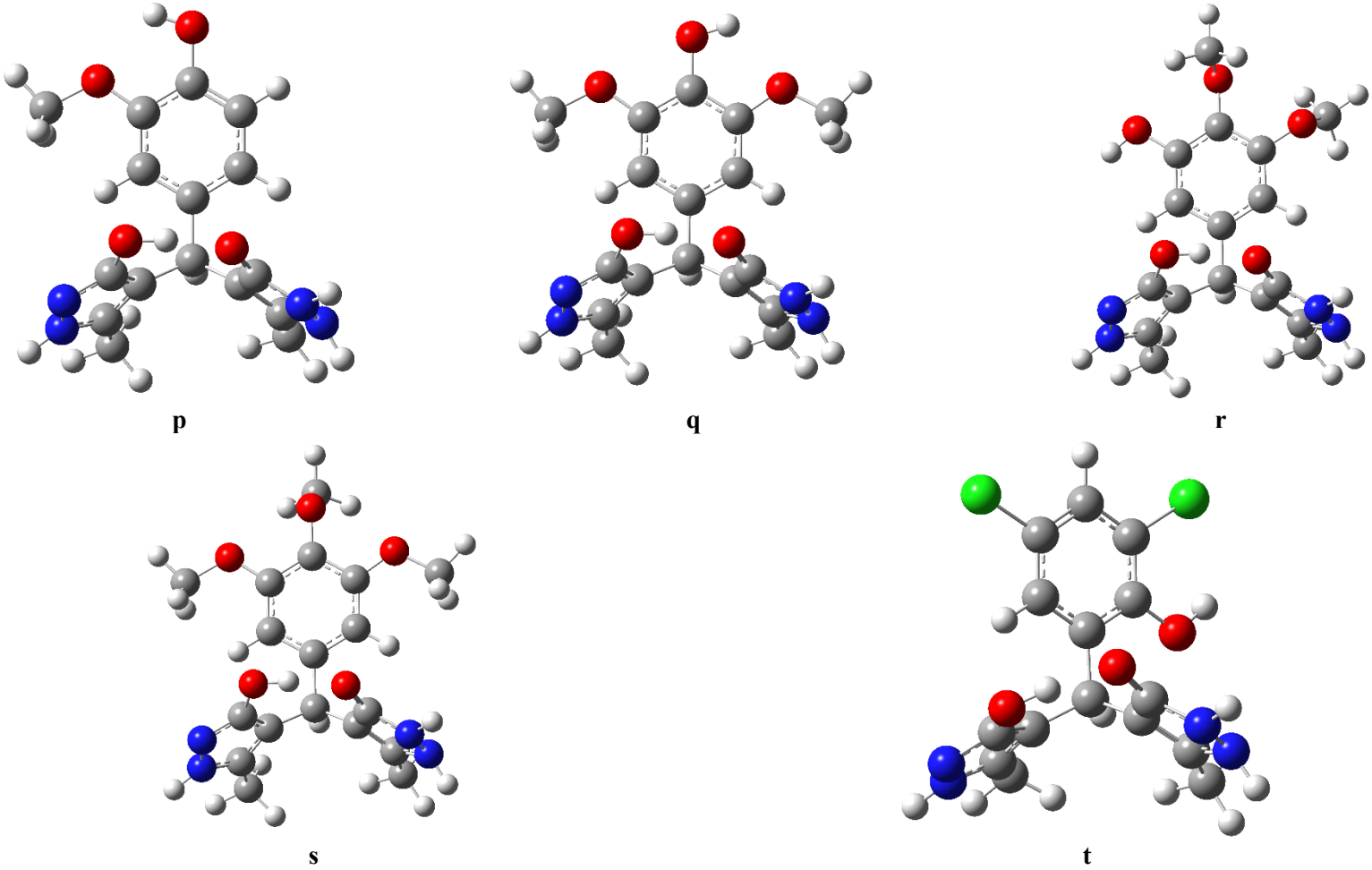


Figure S8. Optimized geometries of compounds **p–t** in water.

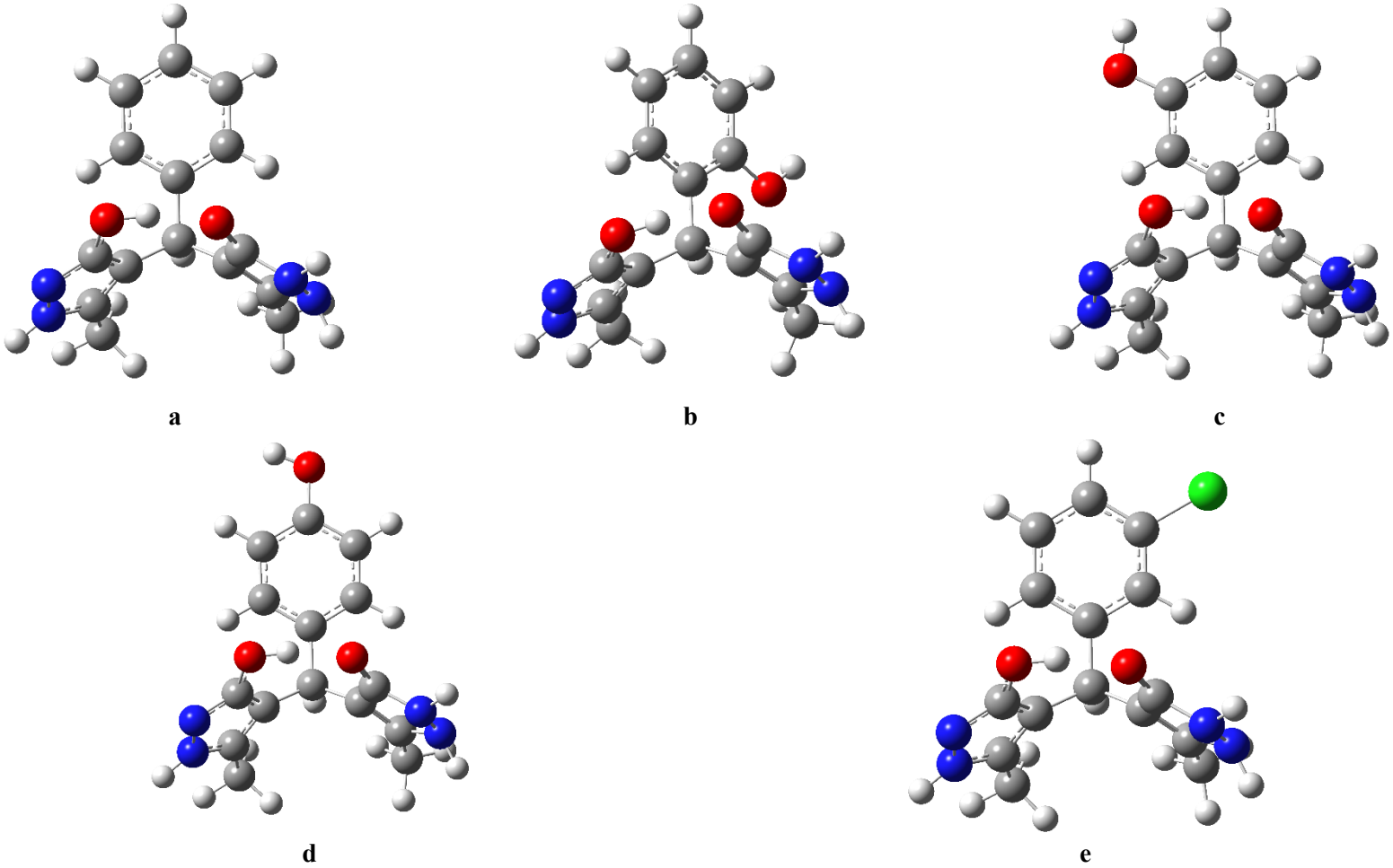


Figure S9. Optimized geometries of compounds **a–e** in benzene.

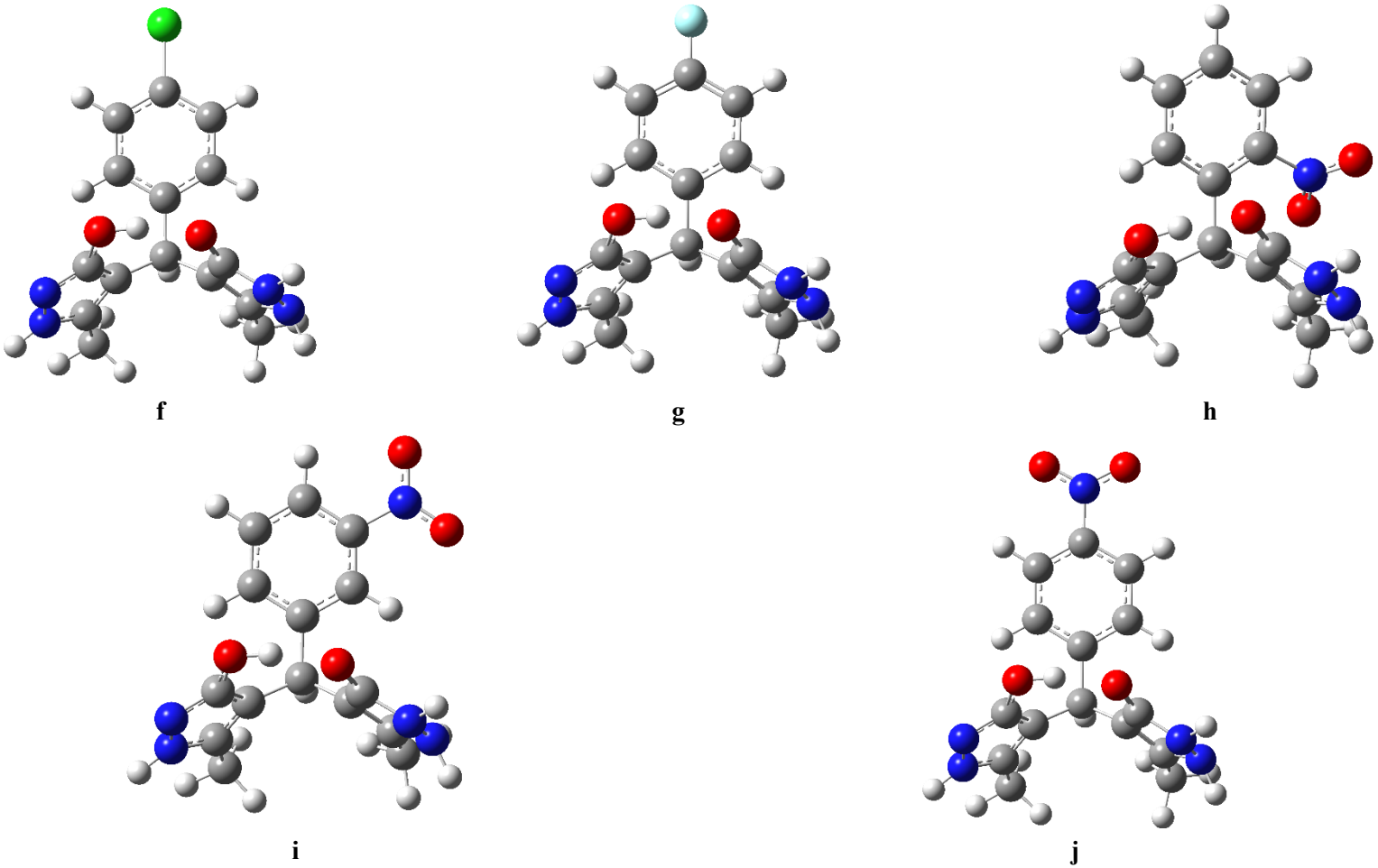
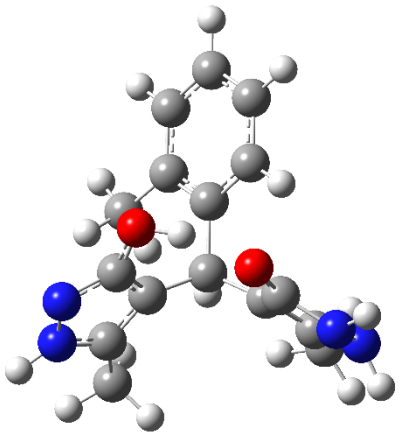
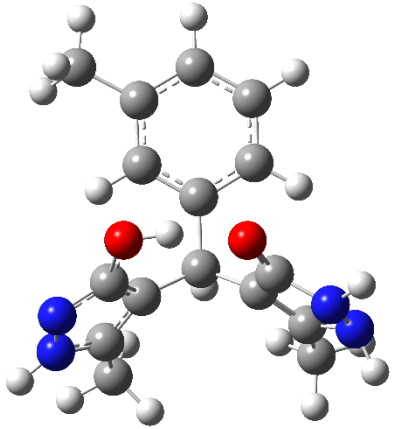


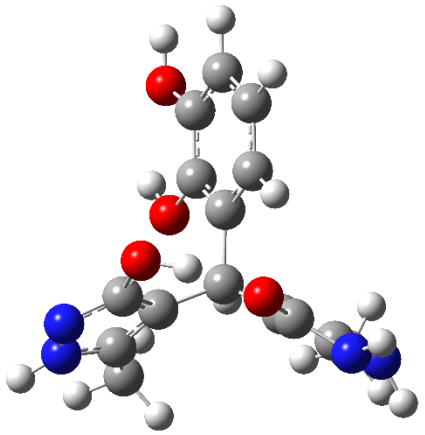
Figure S10. Optimized geometries of compounds **f–j** in benzene.



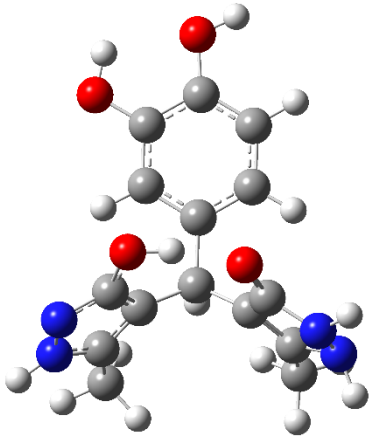
k



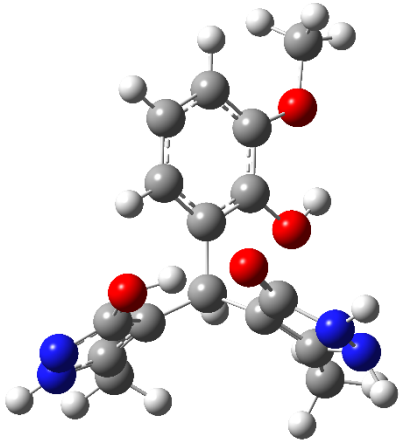
l



m



n



o

Figure S11. Optimized geometries of compounds **k–o** in benzene.

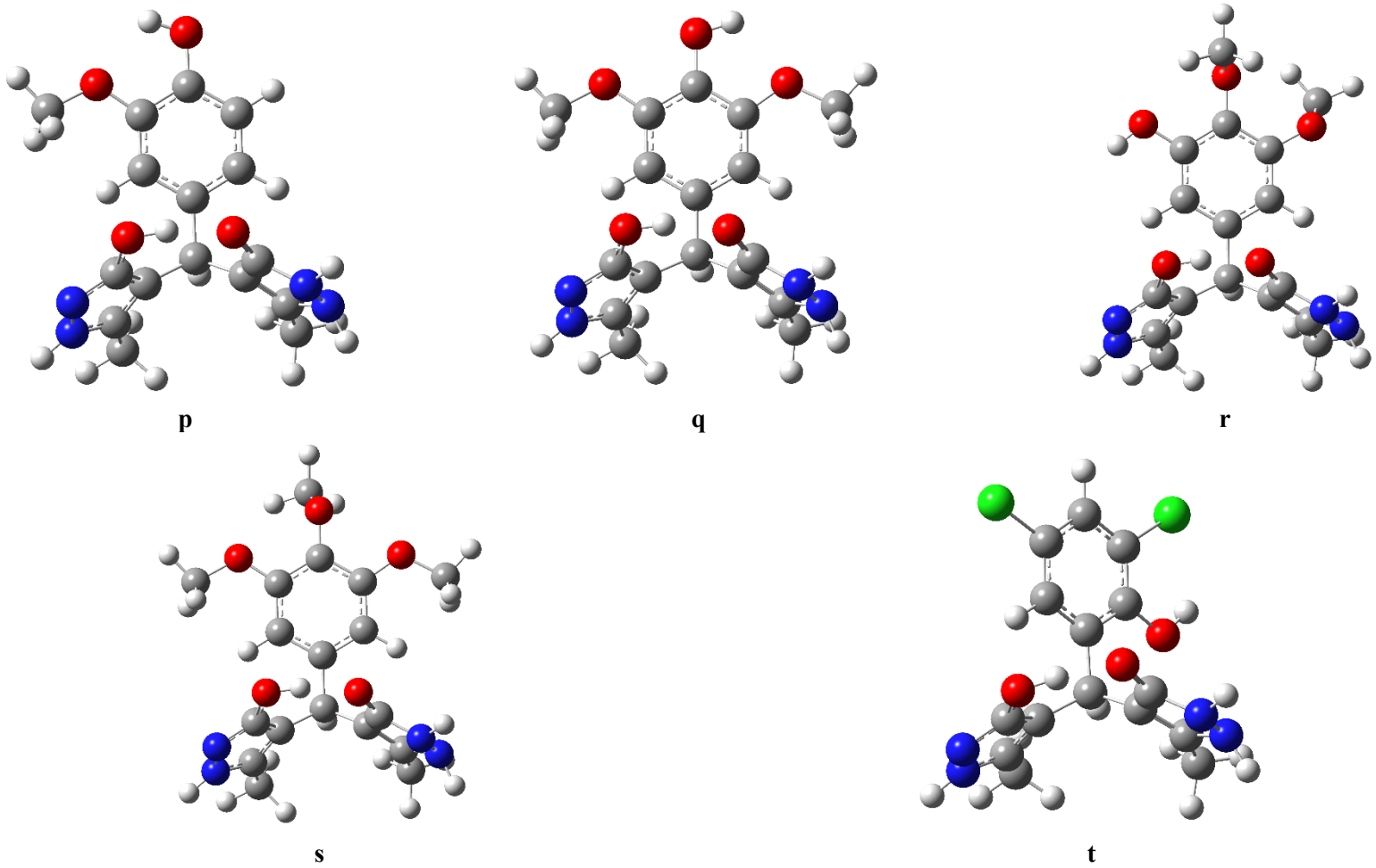


Figure S12. Optimized geometries of compounds **p–t** in benzene.